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Bounds to Truncation Errors in Biorthogonal Polynomial Approximations, With Illustrative Applications to Gamma Ray Transport Distributions*

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(January 29, 1971)

Problems of gamma ray and neutron penetration in infinite, homogeneous media can be solved in terms of infinite sums of a certain type of biorthogonal polynomial system. Many calculations have used a few terms, perhaps 4 to 8, successfully due to good apparent convergence. This paper develops expressions for bounds to the truncation error of these finite sums. Examples and applications are given of the functions used to obtain the error bounds.

Key words: Biorthogonal polynomials; gamma ray transport; moment method; neutron transport; polynomial truncation errors; Sievert function.

1. Introduction

There is an important class of radiation transport problems for which it is feasible to calculate spatial moments

$$M_n=\frac{1}{n!}\int_0^\infty dzz^nF(z), \tag{1}$$

or

$$M_n=\frac{1}{n!}\int_{-\infty}^\infty dzz^nF(z), \tag{1'}$$

by numerical integration of a recursive system of Volterra integral equations of the second kind [1, 2].[1] A detailed description of the procedure for obtaining and evaluating these equations is not pertinent to the discussion here; but it is important that accurate calculation is feasible only for a limited number of the moments, say 6 to 10.

In some of these problems every other moment is unobtainable because the recursive system does not reach it; in other problems every other moment vanishes; and in still other problems it turns out to be advantageous to distinguish between even and odd component distributions, both of which utilize alternate moments only. Thus one continually runs into the problem of constructing distributions which depend on a space variable z, while utilizing powers of the variable z^2 through the use of alternate moments.

There is by now a sizeable body of literature on this subject which references [1–13] do not exhaust. Two general approaches to the problem of constructing the distributions have been used,

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[1] Figures in brackets indicate the literature references at the end of this paper.

namely with polynomials and with sums of functions such as exponentials [2]. The latter method has been referred to as "function-fitting," and a variety of algorithms for determining coefficients in such representations have been used.

The problem which has concerned us is the following: Data from "moment" calculations exists, has proven very useful [5–7], and has even been used as a kind of standard against which data from other procedures with known and possibly severe built-in limitations has been compared [8–10]. Yet there has been no way to assess the errors in the data constructed from the moments. Hence the accuracy of these data, although apparently high and generally assumed so, is not firmly established.

This paper is the second in a series which attempts to put such data on a firmer foundation. There appear to be at least four questions which call for study: Let N be the number of moments which an approximation utilizes. Can one be certain of convergence in the limit $N \to \infty$, (1) for polynomial approximations or (2) for specific function fitting algorithms? Likewise, what is the "truncation error" due to use of only a finite set of moments, (3) in polynomial approximations, or (4) in specific function-fitting approximations?

The first paper in this series, reference [4], was a study of the polynomial system, which essentially answered question (1). A few comments about this will be made in the next section. In this second paper we discuss procedures for estimating the truncation error for the polynomial approximations, i.e., question (3). Two approaches are given, of which one is more suited to the radiation transport problems which are our main concern.

We also have ways of getting at answers to both of the questions (2) and (4), and we hope to make these the subject of one or more additional papers. In fact, function-fitting procedures can be more flexible and accurate than polynomial methods. But problems of convergence and estimation of truncation errors for function-fitting approximations are intimately bound up with the properties of related orthogonal functions, and that is the reason for delaying study of function-fitting approximations until the polynomial problems have been considered.

In the next section we identify the pertinent polynomials by giving some of their main properties. Reference should be made to references [1–4], particularly reference [4], for a more complete discussion of the properties reviewed here.

2. U_n^k Polynomial Systems and Approximations

The polynomial representations to which we have referred are usually written

$$F(z) = \sum_{n=0}^{\infty} F_n U_n^k(z), \tag{2}$$

and our interest also lies in truncated approximations to the infinite series. The independent variable in (2) is written z, with $0 \leq z < \infty$; but it may also be $|z|$, with $-\infty < z < \infty$. The U_n^k are biorthogonal to an adjoint set of polynomials which we designate $\hat{U}_n^k$; and the weight function for the system is $z^k e^{-z}$:

$$\int_0^{\infty} dz z^k e^{-z} \hat{U}_n^k(z) U_m^k(z) = \delta_{nm}, \tag{3}$$

where δ_{nm} is Kronecker's delta. The adjoint polynomials, $\hat{U}_n^k$, are functions of z^2 rather than z or $|z|$. The two sets, U_n^k and $\hat{U}_n^k$, satisfy adjoint *third* order differential equations, and have been shown to be the only biorthogonal polynomials obeying differential equations of this order [3]. We also note that generating functions for the U_n^k are elementary [4],

$$(\sqrt{1-q})^{-k-1} \exp\left(z - z/\sqrt{1-q}\right) = \sum_{n=0}^{\infty} q^n U_n^k(z); \tag{4}$$

and that while generating functions for the $\hat{U}_n^k$ can likewise be written in closed form, only the cases $k=0$, 1 are as simple as (4) [4]:

$$(1-q)^{-1}\cos\left[z\sqrt{q/(1-q)}\right]=\sum_{n=0}^{\infty}q^n\hat{U}_n^0(z),$$

$$[q(1-q)]^{-1/2}\sin\left[z\sqrt{q/(1-q)}\right]=\sum_{n=0}^{\infty}q^n\hat{U}_n^1(z). \tag{4'}$$

Generally speaking, convergence of the series in eq (2) appears to be rapid enough for many important practical problems. Typically the first four or five terms seem to give impressive accuracy over a wide range of z values, say $0\leq z\lesssim 15$.

The Fourier transforms of the U_n^k and the Laplace transforms of the $\hat{U}_n^k$ are simple power functions in the complex plane and have biorthogonality properties on an appropriate contour. From these functions one can show that convergence of the series (1) depends on the location of the singularities of the Fourier transform of $F(|z|)$ [4]. In the gamma ray and neutron problems of interest, the form of the transport equation leads one to expect the singularities to lie on the real axis to the right of a known point. Convergence is then expected if very simple rules are obeyed in choosing a scale parameter (for z) so that all singularities fall in a hyperbolic-shaped region of the complex plane [4].

This leaves unanswered the question of the size of the truncation error which results from use of a finite rather than infinite sum. Our approach here is to obtain "error limit functions" which enable us to bound the error for all values of z. Our method for developing these functions is simple and not particularly new. Nevertheless, because neither the study of truncation errors nor the use of biorthogonal systems is familiar to many physicists and engineers, we put the problem in a fairly general context and in the process include older material to make the discussion more complete.

3. The Adjoint Function and the Norm

One can often, though not always, construct an adjoint function to $F(z)$ which we designate $\hat{F}(z)$,

$$\hat{F}(z)=\sum_{n=0}^{\infty}F_n\hat{U}_n^k(z). \tag{5}$$

In addition, the number $\|F\|$,[2]

$$\|F\|^2=\int_0^{\infty}dz z^k e^{-z}\hat{F}^*(z)F(z)=\sum_{n=0}^{\infty}|F_n|^2, \tag{6}$$

has the properties of a norm. Since these series may or may not converge depending on the sequence of F_n values, these concepts are useful mainly when (6) converges so that the function has a *finite* norm of this type.

In this connection we can bring out some important ideas by rewriting (2), (5), and (6) with an arbitrary renormalization of the polynomials:

$$F(z)=\sum_{n=0}^{\infty}(c_nF_n)\{c_n^{-1}U_n^k(z)\}, \tag{2'}$$

$$\hat{F}(z)=\sum_{n=0}^{\infty}(c_nF_n)\{c_n\hat{U}_n^k(z)\}, \tag{5'}$$

[2] The asterisk in (6) indicates complex conjugate.

where the subscript indicates a renormalization, and

$$\|F\|_r^2 = \sum_{n=0}^{\infty} |c_n F_n|^2. \tag{6'}$$

A comparison with eq (2) makes it clear that the biorthogonality relation holds for the renormalized polynomials (U_n^k/c_n) because the c_n, c_m in (2) can be canceled for all n and m. Further, the distribution $F(z)$ is not changed by this renormalization. But the adjoint function and the norm *are* changed, hence the use of the subscript r in (5′) and (6′). If the constants c_n decrease with n, it is possible for $\|F\|_r$ to be finite when $\|F\|$ is not. Correspondingly, the series for $\hat{F}_r(z)$ may converge where $\hat{F}(z)$ does not.

Before proceeding further, we should note that this discussion, and the discussion to follow, applies to orthogonal as well as biorthogonal systems. But the indicated renormalization generates a difference between two sets of functions which would otherwise be identical for the orthogonal case. Hence application of the argument to orthogonal systems involves treating them as two distinct biorthogonal sets.

4. Transformation Kernels

We need to refer to one other type of function before turning our attention to the problem of estimating limits for the error of truncated series. We denote this bivariate function by $T^k(y, z)$,

$$T^k(y, z) = \sum_{n=0}^{\infty} \{c_n^{-1} U_n^k(y)\}\{c_n^{-1} U_n^k(z)\}. \tag{7}$$

This series may diverge. But if integrals over $T^k(y, z)$ converge, one can assign to this function the properties

$$\{c_n^{-1} U_n^k(z)\} = \int_0^{\infty} dy\, y^k e^{-y} T^k(y, z)\{c_n \hat{U}_n^k\} \tag{8}$$

and

$$F(z) = \int_0^{\infty} dy\, y^k e^{-y} T^k(y, z) \hat{F}_r(y). \tag{8'}$$

Hence we refer to T^k as a transformation kernel for the system.

The diagonal case, $T^k(z, z)$, is more useful to us than $T^k(y, z)$, and we give this one-variable function a special notation,

$$[D^k(z)]^2 = T^k(z, z) = \sum_{n=0}^{\infty} \{c_n^{-1} U_n^k(z)\}^2. \tag{9}$$

If this function exists, it is clearly positive; and it is smaller the larger the c_n's.

5. Some Special Properties and Cases

The normalization for the U_n^k polynomials was chosen fortuitously in reference [1]. One can show that for $c_n = 1$, all the $T^k(y, z)$ can be expressed in terms of modified Bessel functions [4]; while for other choices of c_n such simple expressions probably don't exist. Specifically, for $k = 0$,

$$T^0(y, z) = (2/\pi) K_0(\sqrt{y^2 + z^2})\, e^{(y+z)}, \tag{10}$$

and

$$[D^0(z)]^2 = e^{2z}(2/\pi)K_0(z\sqrt{2}). \tag{11}$$

Since K_0 diverges logarithmically as its argument tends to zero, the series expression for these functions converges except for $y=z=0$. Divergence at this point also follows from the asymptotic expression for $U_n^k(0)$: for $n \to \infty$ [4],

$$U_n^k(0) \to A_k \sqrt{n+1}^{(k-1)}, \tag{12}$$

with $A_0 = 1/\sqrt{\pi}$. Further, one expects that the series (2) will converge for all values of z if

$$\sum_{n=0}^{\infty} \frac{1}{\sqrt{n+1}} |F_n| < \infty. \tag{12'}$$

Since this condition is barely more restrictive than the condition that the norm $\|F\|$ be finite, we expect that for $k=0$, the series (2) usually converges for all values of z when the norm defined by (6) is finite.

For $k \geq 1$, the T^k and D^k are more complicated:

$$[D^1(z)]^2 = \frac{1}{\pi} K_2(z) e^{2z},$$

$$[D^2(z)]^2 = \frac{1}{\pi}\left\{\frac{1}{2}K_4 - \frac{\sqrt{2}}{z}K_3 + \frac{1}{z^2}K_2\right\}e^{2z},$$

$$[D^3(z)]^2 = \frac{1}{\pi}\left\{\frac{1}{4}K_6 - \frac{3/\sqrt{2}}{z}K_5 + \frac{9/2}{z^2}K_4\right\}e^{2z},$$

$$[D^4(z)]^2 = \frac{1}{\pi}\left\{\frac{1}{8}K_8 - \frac{3/\sqrt{2}}{z}K_7 + \frac{21/2}{z^2}K_6 - \frac{9\sqrt{2}}{z^3}K_5 + \frac{9/2}{z^4}K_4\right\}e^{2z}$$

$$T^k = e^{(y+z)} \frac{\partial^2}{\partial y \partial z}\{e^{-(y+z)}T^{k-1}\}. \tag{13}$$

Divergence for $z \to 0$ occurs for all k, and becomes progressively stronger as k increases. In fact, to guarantee convergence at $z=0$ in (7), it is necessary to choose c_n values which tend to ∞ as

$$c_n = \sqrt{n+1}^{k+\epsilon}, \qquad \epsilon > 0. \tag{14}$$

This follows from eq (12). Basically, this factor compensates for weight functions which include the factor z^k, a factor diminishing the amount of information about z near zero which the moments contain. In any case, use of (14) or a different choice which similarly assigns values other than unity to the c_n means that T^k and D^k are not obtainable in such an attractive form as (10) and (13). Such choices also place greater demands on the convergence of the F_n's, if c_n increases without limit.

6. Expressions Bounding the Truncation Error

Our approach to the problem of bounding the truncation error makes use of the Schwarz inequality,

$$\left(\sum_{n=0}^{\infty} f_n g_n\right)^2 \leq \left(\sum_{n=0}^{\infty} |f_n|^2\right)\left(\sum_{n=0}^{\infty} |g_n|^2\right). \tag{15}$$

We write the truncated approximation to (2) in the form

$$F_N(z) = \sum_{n=0}^{N-1} (c_n F_n)\{c_n^{-1} U_n^k(z)\}. \tag{16}$$

Let us also define two infinite sequences, one for coefficients and the other for polynomials. The rules which we follow are as follows:

$$\bar{F}_n = \begin{matrix} F_n, & n < N, \\ 0, & n \geq N, \end{matrix} \tag{17}$$

$$\bar{U}_n^k = \begin{matrix} U_n^k, & n < N, \\ 0, & n \geq N. \end{matrix} \tag{17'}$$

We can then write the truncated series in alternative forms,

$$F_N(z) = \sum_{n=0}^{\infty} (c_n \bar{F}_n)\}c_n^{-1} U_n^k(z)\}, \tag{18}$$

$$F_N(z) = \sum_{n=0}^{\infty} (c_n F_n)\{c_n^{-1} \bar{U}_n^k(z)\}. \tag{18'}$$

If we subtract (18) and (18′) from (2′), and apply the Schwarz inequality, we obtain the expressions we seek,

$$|F - F_N| \leq \|F - F_N\|_r D^k(z), \tag{19}$$

and

$$|F - F_N| \leq \|F\|_r D_N^k(z), \tag{19'}$$

where in agreement with eq (9),

$$\{D_N^k(z)\}^2 = \sum_{n=N}^{\infty} \{c_n^{-1} U_n^k(z)\}^2. \tag{20}$$

One should note here that (19) and (19′) are by no means the only such inequalities which can be written. One can modify (17) and (17′) in many ways, each leading to an inequality. But the expressions written above represent limiting cases of greater interest than some of the other options.[2a]

By and large, we would expect (19) to be of greatest usefulness when the function being approximated is exactly known, perhaps through an expression which gives the F_n for all values of n. Under these circumstances, the norm of the difference function, $\|F - F_N\|_r$, can be determined with high accuracy and certainty, and simple expressions for an upper bound can be derived.

Alternatively, we would expect (19′) to be more useful when the function being approximated is known only in regards to some very general properties, such as asymptotic trends or discontinuous or singular behavior. Under these circumstances the norm of the difference function cannot be accurately known. One may have only some guidance on expected trends with large values of n of the coefficients F_n together with the sequence of estimates of the norm provided by the terms up to the index of truncation. Even though this information is incomplete, it still permits *estimates* of error bounds for all values of z through an estimation of the likely magnitude of a single number. This information is useful, the more so in combination with the sequence of approximations obtained by changing the index of truncation.

The case (19′) is of greater use in the calculation of gamma ray and neutron distributions, in which we have a particular interest.

[2a] Note that D_N^k can replace D^k in (19) to give a sharper form.

In a general way, one can say that the c_n's provide a mechanism for translating some very general information about the function $F(z)$ into a reduction of the error bounds of a truncated approximation. If one knows that the F_n's decrease strongly with large n—and this information would follow from location and type of singularities of the Fourier transform—then one can use c_n values which increase rather strongly with increasing values of n. A proper choice would result in only a small increase in either $\|F-F_N\|_r$ or $\|F\|_r$, while it would decrease D^k and D_N^k substantially for all values of z. The result is therefore a narrowing of the estimated bounds for the truncation error.

6.1. Error Limit Functions

Table 1 presents examples of "error limit functions." The second column gives D^k, and the remaining columns give ratios D_N^k/D^k. These data, somewhat augumented, are also presented in figure 1. For this case and for others to be mentioned, the c_n have the form

$$c_n=(n+1)^{j/4}, \tag{21}$$

and in table 1, and figure 1, the results are for $j=2$.

Note that there are N minima in figure 1, and that they are spaced more widely apart at larger z. Note also that from one value of N to the next a drop by perhaps a factor of $\sqrt{2}$ occurs, while the final rise to unity advances by about $\Delta z=4$ to the right.

TABLE 1. *Values for the functions* $D^0(z)$ *and* D_N^0/D^0 *given by eqs (9) and (20), using the expression (21) for* c_n *with* $j=2$

z	D^0	$N=1$	2	4	7
0.00	1.124	0.4561	0.3302	0.2293	0.1643
.25	1.048	.2997	.1607	.06876	.02627
.50	1.019	.1903	.07817	.05558	.05302
.75	1.009	.1334	.1007	.09329	.06760
1.00	1.011	.1492	.1492	.1094	.06037
1.50	1.040	.2735	.2142	.09805	.02875
2.00	1.091	.3993	.2332	.06267	.02468
3.00	1.246	.5970	.1860	.06151	.03530
4.00	1.470	.7331	.1308	.09293	.01661
5.00	1.770	.8252	.2071	.07939	.02489
6.00	2.163	.8867	.3439	.05320	.02746
7.00	2.671	.9273	.4789	.07480	.01733
8.00	3.328	.9538	.5971	.1147	.01821
10.00	5.264	.9818	.7736	.1369	.02865
12.00	8.488	.9930	.8810	.1020	.01864
14.00	13.88	.9974	.9408	.1970	.03812
16.00	22.94	.9990	.9719	.3750	.03721
18.00	38.24	.9997	.9872	.5499	.03231
20.00	64.19	.9999	.9944	.6953	.06604
22.00	108.4	1.000	.9976	.8047	.08923
25.00	239.8	1.000	.9994	.9084	.07327
30.00	917.8	1.000	.9999	.9790	.2758

Figure 2 shows the effect of changing the value of j in (21). When j is increased by unity, the curves are reduced by a factor which is much larger at small z than large. The positions of the minima are essentially unchanged.

Figure 3 illustrates changes when k is increased. The main effects are as follows: (a) there is is a shift of all minima to the right, this shift being larger for large z than for small z; and (b) there is a substantial increase in D_N^k/D^k, particularly for values of z near zero. This increase reflects the reduction of the small z region's contribution to the polynomial coefficients, due to the factor

of z added to the weight function. Beyond the small z region, equal increases in k and j have nearly compensating effects on the ordinates of corresponding maxima and minima.

Figure 4 shows a number of functions $D^k(z)$, for different values of k and j. The *trend* with z does not change very much, although the curves are reduced at large z when j is increased. Increases in the value of k show a correspondingly stronger divergence for $z \to 0$. Beyond this one might say that the main effect of unit increase in k is a shift of the curve to the right by about $\Delta z = 1$.

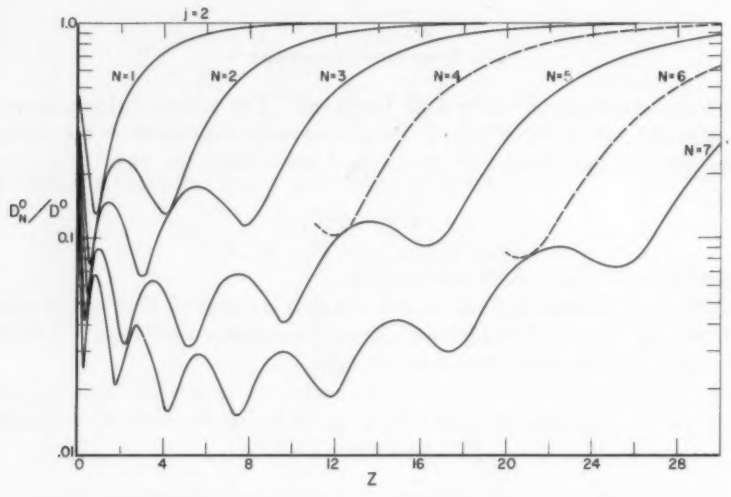

FIGURE 1. *Data from table 1, for functions defined by eqs (9) and (20), with* $c_n = \sqrt{n+1}$ *and* $k = 0$.

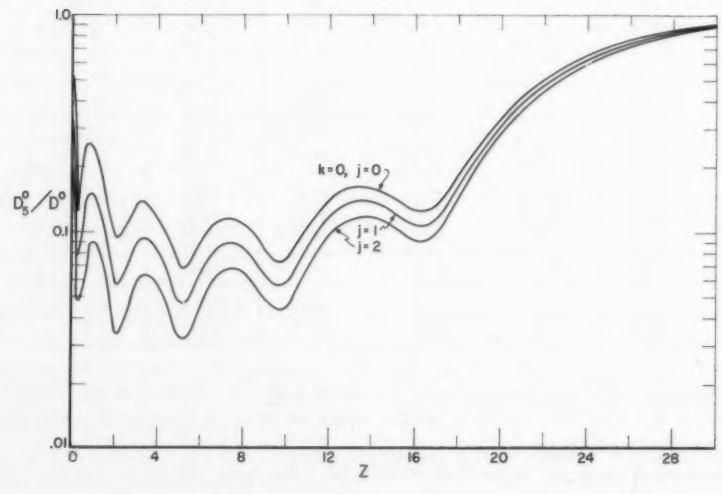

FIGURE 2. *The ratios* D^0_N/D^0, *for* $N = 5$, *and* $c_n = (\sqrt[4]{n+1})^4$.

Data for different values of j are compared.

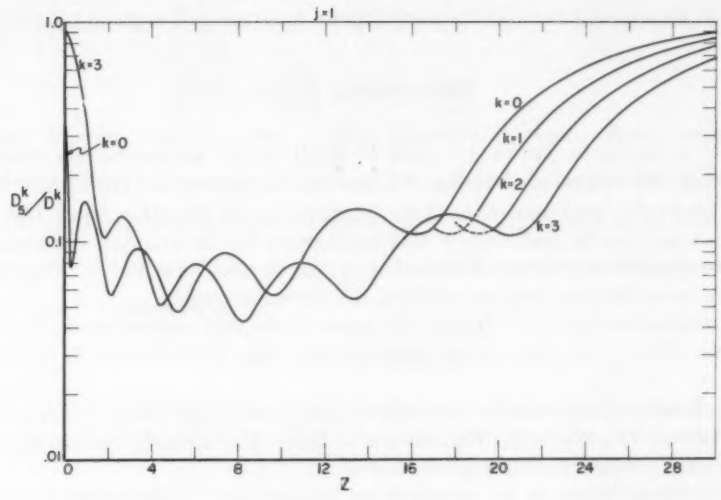

FIGURE 3. *The ratios* D_N^k/D^k, *for* $N=5$ *and* $c_n=(\sqrt[4]{n+1})^{k+1}$.

Data for different values of k are compared.

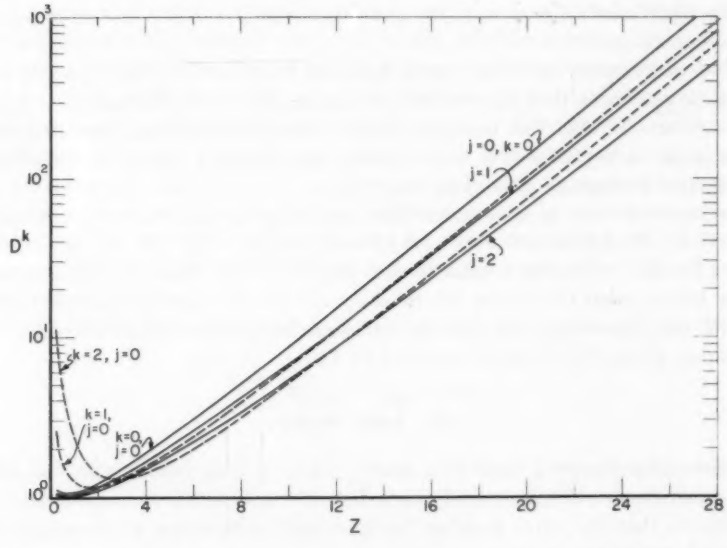

FIGURE 4. *The functions* $D^k(z)$, *for several values of* k, *using* $c_n=(\sqrt[4]{n+1})^j$, *with* j *also taking different values.*

6.2. Fractional Error Limits

Using (19) and (19′), we write the ratio of error limits to function $F(z)$ being approximated as follows,

$$\frac{|F-F_N|}{F(z)} \leq Eb(z)\left\{\frac{\|F-F_N\|_r}{\|F\|_r}\right\}; \tag{22}$$

$$\leq Eb(z)\left\{\frac{D_N^k(z)}{D^k(z)}\right\} \tag{22′}$$

where $Eb(z)$ will be referred to as an "error buildup" function and is given by

$$Eb(z) = D^k(z)\,\frac{\|F\|_r}{F(z)}. \tag{23}$$

The ratio D_N^k/D^k is shown in figures 1–3, and depends on the approximation system but not on the function being approximated. Further, its general characteristics are largely determined by the number of moments used and other input information. On the other hand, $Eb(z)$ depends on the function $F(z)$ and can be modified by making changes in this function of a manipulative type, which do not necessarily represent additional input information. Further, if $F(z)$ cannot be well-represented, the error buildup function exhibits the situation clearly.

Thus the representation (22′) divides the error limits into system-dependent and function-dependent parts. (This is not true if use of (19) rather than (19′) results in replacing D_N^k/D^k by $\|F-F_N\|_r/\|F\|_r$.)

Clearly the fractional error limits cannot be made small unless $Eb(z)$ is kept within a reasonable range of values. The trend of $D^k(z)$ shown in figure 4 is strongly increasing, hence $F(z)$ is ideally also a rather strongly increasing function of z.

To illustrate these ideas let us consider the simple case $F(z)=1$. Since the norm of this function is unity for all values of k, $Eb(z)$ is given by $D^k(z)$. From figure 4, using $k=0$, $j=0$, one thus obtains a value of 8.6 for Eb at $z=10$, and from calculations similar to those of table 1 we evaluate D_N^k/D at 0.051, so that the fractional error limits are about 8.6×0.051, or about ± 44 percent. On the other hand, if one uses (19) and (23), since $\|F-F_N\|$ is known to be zero for $N\geq 1$, the error limits vanish.

For contrast we consider next the simple function $F(z)=e^{z/5}/(1.25)^{k+1}$, again with $k=0$, and $j=0$. From eq (4) one sees that $F_n=(-9/16)^n$, hence $\|F\|_r=\sqrt{1.46}$; and $\|F-F_N\|_r$, with $N=7$, has the value $\sqrt{1.46}\cdot 0.0178$. The function $Eb(z)$ turns out to be less than three out to a value of z at least as great as $z=16$, and it is no greater than about 6 out to $z=25$. (These comments omit the logarithmic divergence *very* close to $z=0$).

These results enable us to determine that according to eq (19), the error limits are below 5 percent out to $z=16$, and below about 10 percent out to $z=25$. On the other hand, by use of (19′), and data for the $j=0$ case similar to that of table 1 and figure 1, we determine that error limits fluctuate below about 15 percent out to about $z=16$, but rise to about 50 percent at $z=25$.

In a general way, one might say that the narrower limits given by (19) are due to use of more refined information about $F(z)$ than is required by (19′).

6.3. Scale Factors

The two functions $F(z)=1$, and $F(z)=e^{z/5}/(1.25)^{k+1}$, can be regarded as differing mainly in regards to scale factor. If we multiply both by e^{-z} we see this more clearly. The preceding discussion suggests that the error buildup function can be modified to advantage by changes in scale factor which are very easy to make.

To state this in general form, we depart from the practice to this point of using only e^{-z} as weight factor. More generally, we represent a function $F(z)$ with the approximation

$$F(z) \approx \sum_{n=0}^{N} c_n F_n \left\{\frac{1}{c_n}\, U_n^k(z/\xi)\right\}, \tag{24}$$

where the constants c_n have the interpretation previously given, and the scale factor ξ is arbitrary. Expansion coefficients F_n are given by

$$\int_0^\infty d(z/\xi)\hat{U}_n^k(z/\xi)\,(z/\xi)^k e^{-z/\xi}F(z). \tag{25}$$

If the distribution $F(z)$ has an asymptotic trend which is exponential, with coefficient $(\mu_m - 1/\xi) \neq 0$,

$$F(z) \to f(z)e^{-\mu_m z + z/\xi},$$

where f is some function which is weaker than exponential, then a finite norm requires that $\frac{1}{\xi} < \mu_m \cdot \sqrt{2}$. Beyond this, however, the choice of ξ is a practical matter, affected by rate of convergence and the resulting size of $Eb(z)$. It turns out that $Eb(z)$ is apt to be better behaved if ξ is chosen a little smaller than $1/\mu_m$, say $\xi \sim \frac{.8}{\mu_m}$. But other considerations can sharpen the selection of scale factor considerably.

6.4. Trends Near Zero

It may happen that the trend of $F(z)$ near zero is known precisely. One can then approximate a modified function, $F(z) - C(z)$, where $C(z)$ has the known trend for $z \to 0$, tends to zero more strongly than $F(z)$ for $z \to \infty$, but is otherwise arbitrary. The combination $F(z) - C(z)$ can then be proportional to z or z^2 for small z, so that approximation by U_n^1 or U_n^2 polynomials is appropriate, rather than U_n^0 polynomials.

This situation has many advantages. The U_n^k systems for higher k values are not so accurate for small z, but extend their accuracy considerably farther in the direction of large z values. But if the small values of z cause no problem, due to use of known trends, the accuracy at larger z values is obtained essentially without cost. Use of this additional information thus turns out to give greater accuracy for all z values, small as well as large, as well as narrower bounds on the error.

If, in addition, many moments of the unknown function are available for use, it is possible to omit the lowest moments, while at the same time increasing the value of k even more. This decreases the accuracy for small z values somewhat, but in such a way that the decrease in both accuracy, and knowledge of the accuracy, is not necessarily large enough to be important. At the same time, the approximation for intermediate and large z may be considerably improved. This suggestion of omitting low moments and using large k values was made by E. Morris [13]. Morris did not attempt to obtain a single approximation, but used this approach to extend a low k approximation to much larger z values.

Example 1: The Sievert Integral. Standard tabulations exist of the Sievert integral [14],

$$S(z, \theta) = \int_0^\theta d\phi e^{-z/\cos\phi}, \tag{25}$$

but due to the fact that two variables are involved, additional representations may well prove useful. Hence the evaluation in terms of U_n polynomials is perhaps a nontrivial example of the use of error functions of the type (20′). Writing

$$\cos\theta = \sqrt{1-\beta}$$

and expanding by means of eq (4), we evaluate the integral term by term to obtain:

$$S(z, \theta) = \sum_{n=0}^{\infty} \frac{(\sin\theta)^{2n+1}}{2n+1} e^{-z} U_n^0(z). \tag{26}$$

If we evaluate this expression, using m terms in the series, the error according to eq (19) is governed by the inequalities

$$(\text{Error})^2 \leq \left\{ \sum_{n=m}^{\infty} \frac{(\sin\theta)^{4n+2}}{(2n+1)^2} \right\} \frac{2}{\pi} K_0(z\sqrt{2}), \tag{27}$$

or, say, using $c_n = (2n+1)^{1/4}$,

$$(\text{Error})^2 \leq \left\{ \sum_{n=m}^{\infty} \frac{(\sin\theta)^{4n+2}}{(2n+1)^{3/2}} \right\} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n+1}} \left[e^{-z} U_n^0(z) \right]^2. \tag{27'}$$

Note that the error limit given by (27′) is finite at $z=0$. Writing ν for 3/2 or 2, we have

$$\begin{aligned} \sum_{n=N}^{\infty} \frac{(\sin\theta)^{4n+2}}{(2n+1)^{\nu}} &\leq \frac{(\sin\theta)^{4N+2}}{(2N+1)^{\nu}} \left\{ 1 + \sin^4\theta \int_{N+1/2}^{\infty} dx \, \frac{(2N+1)^{\nu}}{(2x)^{\nu}} \right\}, \\ &\leq \frac{(\sin\theta)^{4N+2}}{(2N+1)^{\nu}} \left\{ 1 + \frac{2N+1}{2(\nu-1)} \sin^4\theta \right\}. \end{aligned} \tag{28}$$

Table 2 gives selected values of the ratio $\|F - F_N\|_r / \|F\|_r$, obtained using (27′) and (28). The latter gives an overestimate which for intermediate values of θ can be up to a factor of 2 too high. The norm ratios of table 2 show that (26) gives very accurate values even with only a few terms, throughout a wide range of z values, provided θ is small, say $\theta < \pi/4$.

The approximations of table 3 are given despite being somewhat unimpressive because they illustrate relationships between errors, error limits, scaled and unscaled approximations, and the two approaches to obtaining error limits. For θ near $\pi/2$, eq (26) has slow convergence due to the "sharp" component with cos ϕ near zero. Table 3 gives a variety of types of data for the worst case,

TABLE 2. *Values of* $\|\mathbf{F} - \mathbf{F}_N\|_r / \|\mathbf{F}\|_r$ *calculated using eq (27′)*

The numbers in parenthesis give approximations in which the numerator of the ratio is obtained using eq (28). (Note that the form A–B means $A \times 10^{-B}$ in the top entries.)

θ	$N=2$		4		6	
0	0		0		0	
15°	1.3–3	(1.4–3)	0.39–5	(0.39–5)	1.3–8	(1.4–8)
30°	1.9–2	(2.1–2)	.77–3	(.94–3)	0.36–4	(.48–4)
45°	0.079	(.11)	.013	(.021)	.0025	(.0046)
60°	.20	(.31)	.075	(.16)	.033	(.070)
75°	.36	(.52)	.23	(.37)	.16	(.29)
90°	.54	(.57)	.46	(.47)	.41	(.42)

TABLE 3. *Fractional error and error limit data for* S(z, π/2)

To obtain the quantities in parenthesis, a scaled function was calculated, with $\xi = 0.8$. This reduces the *Eb* function strongly at large z. N is the number of terms in the approximating series. Data in the "error" column is fractional. Fractional error limits can be obtained by multiplication of *Eb* by D_N^0/D^0.

z	*Eb*		D_4^0/D^0		$N=4$ Error		D_7^0/D^0		$N=7$ Error	
0	0.97	(1.16)	0.366	(0.366)	−0.18	(−0.15)	0.287	(0.287)	−0.14	(−0.11)
0.25	.96	(1.08)	.106	(.079)	−.014	(−.003)	.046	(.047)	.008	(.014)
.50	1.02	(1.11)	.106	(.137)	.04	(.04)	.103	(.120)	.04	(.03)
.75	1.11	(1.16)	.158	(.173)	.06	(.04)	.123	(.112)	.04	(.02)
1.00	1.22	(1.21)	.175	(.168)	.07	(.04)	.105	(.076)	.03	(.01)
1.5	1.48	(1.31)	.148	(.108)	.05	(.01)	.050	(.041)	.002	(−.01)
2	1.76	(1.40)	.095	(.070)	.01	(−.01)	.045	(.060)	−.02	(−.01)
4	3.17	(1.79)	.128	(.106)	−.08	(−.02)	.027	(.038)	.007	(.006)
7	8.09	(2.61)	.098	(.164)	.17	(.05)	.025	(.036)	−.004	(−.008)
10	19.4	(3.69)	.163	(.130)	.29	(−.04)	.038	(.030)	−.07	(.01)
15	91.2	(6.79)	.313	(.640)	4.0	(−.42)	.051	(.052)	.35	(−.03)

$\theta = \pi/2$. Two sets of data, corresponding to 4-term and 7-term approximations, are shown. In all calculations, $k = 0$ and $j = 1$. Data (in parenthesis) are also given for another calculation in which a scaling of $\xi = 0.8$ was used to reduce both the error and the error limits. The two factors giving error limits, $Eb(z)$ and D_N^0/D^0, are presented separately.

Comparison of the data in parenthesis for Eb with that not in parenthesis demonstrates the reduction of this factor which the scaling brings about. The other factor, D_N^0/D^0, is not greatly affected by the scaling except that the eventual rise to unity is moved to smaller z value, as already noted.

Errors given for the scaled approximation are almost uniformly smaller, and this is especially marked for large z values.

Error limits calculated by multiplying Eb by D_N^0/D^0 are usually two or more times larger than the actual errors. The pattern of error sizes shows a marked tendency to follow the pattern of error-limit sizes. This is expected, because both are affected by the maxima and minima of the first few polynomials not included in the approximation.

Example 2: Point and Plane Isotropic Gamma Ray Distributions. In the calculation of gamma ray distributions, one can classify components of the distribution by an index which gives the number of scattering interactions that the photons have had with atoms of the surrounding material. Thus one speaks of unscattered, once-scattered, twice-scattered, etc., components. The multiply-scattered component is the sum of all components scattered at least twice.

The advantage of this classification system is in part due to the fact that unscattered and once-scattered components can be described by analytic expressions for many configurations. The multiply-scattered component represents the primary objective of the polynomial representation referred to in this paper; and for a configuration in which the photon source is idealized as a point, the multiply-scattered component is known to vary approximately as z^2 near the source.

One procedure for accurate calculation of distributions is thus to determine unscattered and once-scattered components by direct functional evaluation and quadrature, and to evaluate the multiply-scattered component by polynomial representation. Due to the known z^2e^{-z} dominance in the spatial trend of this component, we have used U_n^2 polynomials. It turns out that the z-dependence of the function multiplying z^2e^{-z}, which is our $F(z)$ to be determined, has a trend which produces an error buildup ratio (22′) which does not increase satisfactorily. Hence we have used a value $\xi = 1/1.2$ to decrease the error limits. Because the norm is not known, but the convergence of the norm appears to be very good, we have used the largest of the sequence of norm values shown in table 4, together with an error limit expression of the type (19′) with $c_m = \sqrt[4]{m+1}$, i.e., $j = 1$, to give the values in the next to last error column of table 4.[3]

Table 4 shows unscattered and once-scattered components as well as the multiply-scattered component. The sum of all components is given in the "Total" column. The last column on the right gives an indication of the truncation error, through use of the difference between approximations using 6 and 8 moments. Both error columns are divided by "Total", rather than by the multiply-scattered result. This explains the tendency for errors to vanish as $z \to 0$, since the "Total" contains the unscattered component, which is finite in this limit.

The data of table 5 were obtained from the data of table 4 by numerical integration, using

$$I_{PLI}(z) = \frac{1}{2}\int_{|z|}^{\infty} \frac{dr}{r} I_{PTI}(r), \tag{30}$$

[3] We use a smaller value of j than (14) would suggest because a factor z^2 is applied to the error limits here. Resulting convergence to zero shown on the table at $z = 0$ is conjectured, rather than proven.

TABLE 4. *Gamma ray energy deposition from a point isotropic, Cs-137 source in air*

The first two columns give distance in g/cm² and in feet. The next three columns give unscattered, once scattered, and multiply scattered components, respectively. The column labeled "Estimated Err Lim" gives an estimated fractional error limit to the "Total" column. The final column gives the fractional contribution of the last two terms in the series. For this calculation a total of 8 terms was used in the expansion. Integration of the total with respect to distance (in g/cm²) gives unity.

Energy deposition in air

g/cm²	Feet	0 Scat	1 Scat	2+ Scat	Scat/Unscat	Total	Estimated Err Lim	Final Two Terms
0.0000	0.00	2.943−02	0.000	0.000	0.000	2.943−02	0.000	0.000
.1102+00	3.00	2.919−02	2.189−04	2.049−06	7.571−03	2.941−02	7.610−04	4.147−06
.1205+00	3.28	2.916−02	2.389−04	2.447−06	8.274−03	2.940−02	9.063−04	4.946−06
.1469+00	4.00	2.910−02	2.898−04	3.628−06	1.008−02	2.940−02	1.335−03	7.314−06
.2204+00	6.00	2.894−02	4.288−04	8.098−06	1.510−02	2.938−02	2.925−03	1.620−05
.2938+00	8.00	2.878−02	5.643−04	1.428−05	2.011−02	2.935−02	5.063−03	2.834−05
.3673+00	10.00	2.861−02	6.967−04	2.214−05	2.512−02	2.933−02	7.702−03	4.358−05
.4407+00	12.00	2.845−02	8.262−04	3.162−05	3.015−02	2.931−02	1.080−02	6.176−05
.5509+00	15.00	2.821−02	1.015−03	4.881−05	3.771−02	2.927−02	1.620−02	9.420−05
.7346+00	20.00	2.781−02	1.317−03	8.506−05	5.041−02	2.922−02	2.693−02	1.609−04
.9182+00	25.00	2.742−02	1.604−03	1.303−04	6.324−02	2.916−02	3.931−02	2.414−04
.1102+01	30.00	2.704−02	1.877−03	1.839−04	7.622−02	2.910−02	5.285−02	3.338−04
.1205+01	32.80	2.682−02	2.024−03	2.174−04	8.355−02	2.907−02	6.079−02	3.899−04
.1469+01	40.00	2.628−02	2.384−03	3.141−04	1.027−01	2.898−02	8.180−02	5.466−04
.2204+01	60.00	2.484−02	3.265−03	6.529−04	1.577−01	2.875−02	1.385−01	1.040−03
.2938+01	80.00	2.347−02	3.993−03	1.073−03	2.158−01	2.853−02	1.834−01	1.556−03
.3673+01	100.00	2.218−02	4.593−03	1.550−03	2.770−01	2.832−02	2.109−01	2.036−03
.4407+01	120.00	2.096−02	5.085−03	2.066−03	3.412−01	2.811−02	2.206−01	2.441−03
.5509+01	150.00	1.925−02	5.652−03	2.876−03	4.430−01	2.778−02	2.076−01	2.860−03
.7346+01	200.00	1.671−02	6.238−03	4.230−03	6.265−01	2.718−02	1.491−01	3.013−03
.9182+01	250.00	1.450−02	6.493−03	5.486−03	8.260−01	2.648−02	1.156−01	2.564−03
.1102+02	300.00	1.259−02	6.518−03	6.579−03	1.040+00	2.568−02	1.428−01	1.696−03
.1205+02	328.00	1.163−02	6.457−03	7.107−03	1.166+00	2.519−02	1.650−01	1.103−03
.1469+02	400.00	9.485−03	6.136−03	8.184−03	1.510+00	2.381−02	2.023−01	−5.241−04
.2204+02	600.00	5.384−03	4.701−03	9.310−03	2.602+00	1.940−02	1.689−01	−3.517−03
.2938+02	800.00	3.056−03	3.265−03	8.649−03	3.898+00	1.497−02	1.002−01	−2.931−03
.3673+02	1000.00	1.735−03	2.152−03	7.221−03	5.403+00	1.111−02	1.182−01	−3.546−04
.4407+02	1200.00	9.849−04	1.374−03	5.635−03	7.117+00	7.994−03	1.193−01	2.080−03
.5509+02	1500.00	4.212−04	6.746−04	3.566−03	1.007+01	4.662−03	6.924−02	3.141−03
.7346+02	2000.00	1.023−04	1.936−04	1.434−03	1.591+01	1.730−03	9.283−02	−6.928−04
.9182+02	2500.00	2.483−05	5.308−05	5.154−04	2.290+01	5.933−04	5.801−02	−3.566−03
.1102+03	3000.00	6.028−06	1.415−05	1.733−04	3.110+01	1.935−04	9.285−02	−1.135−03
.1469+03	4000.00	3.553−07	9.570−07	1.731−05	5.140+01	1.862−05	9.281−02	5.780−03
.1807+03	4920.00	2.627−08	7.747−08	1.875−06	7.432+01	1.979−06	1.419−01	−3.699−03
.1939+03	5280.00	9.480−09	2.879−08	7.703−07	8.429+01	8.086−07	1.288−01	−9.792−03
.2327+03	6336.00	4.769−10	1.557−09	5.439−08	1.173+02	5.642−08	3.542−01	−1.410−02
.2909+03	7920.00	5.380−12	1.904−11	9.471−10	1.796+02	9.715−10	8.743−01	6.110−02
.3394+03	9240.00	1.282−13	4.775−13	3.001−11	2.378+02	3.061−11	1.860+00	1.716−01
Norm sequence:	0.1929−01	0.2001−01	0.2041−01	0.2043−01	0.2045−01	0.2045−01	0.2046−01	0.2046−01

where I_{PLI} and I_{PTI} are point and plane isotropic source distributions respectively.[4] This integration was also performed using data for error limits and the difference between approximations; in this way the results shown in the error columns of table 5 were obtained.[5]

[4] This elementary integral occurs when the plane isotropic source is considered to be a uniform distribution of point isotropic sources over the plane.

[5] Note that if the error in I_{PTI} is designated by δI_{PTI} while the error limit is L, with $L \geq 0$, then

$$\int \frac{dr}{r} L \geq \left| \int \frac{dr}{r} \delta I_{PTI} \right|;$$

and integration of L thus gives a limit for $|\delta I_{PLI}|$.

TABLE 5. *Gamma ray energy deposition from a plane isotropic* Cs-*137 source in air.*

[Interpretation of the columns is the same as in table 4.]

		Energy deposition in air						
g/cm²	Feet	0 Scat	1 Scat	2+ Scat	Scat/Unscat	Total	Estimated Err Lim	Final Two Terms
0.1102+00	3.00	6.181−02	9.241−03	9.142−03	2.974−01	8.019−02	1.210−01	7.170−04
.1205+00	3.28	6.051−02	9.230−03	9.142−03	3.036−01	7.888−02	1.230−01	7.288−04
.1469+00	4.00	5.762−02	9.204−03	9.142−03	3.184−01	7.596−02	1.277−01	7.565−04
.2204+00	6.00	5.173−02	9.132−03	9.140−03	3.532−01	7.000−02	1.383−01	8.197−04
.2938+00	8.00	4.758−02	9.061−03	9.139−03	3.825−01	6.578−02	1.468−01	8.705−04
.3673+00	10.00	4.438−02	8.991−03	9.137−03	4.085−01	6.251−02	1.541−01	9.137−04
.4407+00	12.00	4.178−02	8.922−03	9.134−03	4.322−01	5.983−02	1.605−01	9.515−04
.5509+00	15.00	3.862−02	8.820−03	9.130−03	4.648−01	5.657−02	1.687−01	1.001−03
.7346+00	20.00	3.459−02	8.653−03	9.121−03	5.139−01	5.236−02	1.801−01	1.068−03
.9182+00	25.00	3.150−02	8.490−03	9.109−03	5.586−01	4.910−02	1.892−01	1.122−03
.1102+01	30.00	2.902−02	8.332−03	9.095−03	6.005−01	4.645−02	1.966−01	1.165−03
.1205+01	32.80	2.782−02	8.245−03	9.086−03	6.230−01	4.515−02	2.002−01	1.185−03
.1469+01	40.00	2.518−02	8.026−03	9.060−03	6.785−01	4.227−02	2.075−01	1.225−03
.2204+01	60.00	1.999−02	7.457−03	8.965−03	8.214−01	3.642−02	2.182−01	1.260−03
.2938+01	80.00	1.651−02	6.937−03	8.843−03	9.555−01	3.229−02	2.194−01	1.208−03
.3673+01	100.00	1.397−02	6.457−03	8.698−03	1.085+00	2.912−02	2.153−01	1.087−03
.4407+01	120.00	1.200−02	6.016−03	8.535−03	1.213+00	2.655−02	2.089−01	9.105−04
.5509+01	150.00	9.754−03	5.417−03	8.261−03	1.402+00	2.343−02	1.993−01	5.725−04
.7346+01	200.00	7.163−03	4.559−03	7.754−03	1.719+00	1.948−02	1.924−01	−9.815−05
.9182+01	250.00	5.421−03	3.847−03	7.213−03	2.040+00	1.648−02	1.969−01	−7.855−04
.1102+02	300.00	4.185−03	3.252−03	6.663−03	2.369+00	1.410−02	2.025−01	−1.393−03
.1205+02	328.00	3.645−03	2.963−03	6.358−03	2.557+00	1.297−02	2.027−01	−1.676−03
.1469+02	400.00	2.597−03	2.339−03	5.599−03	3.056+00	1.054−02	1.941−02	−2.147−03
.2204+02	600.00	1.101−03	1.221−03	3.792−03	4.553+00	6.114−03	1.498−01	−1.720−03
.2938+02	800.00	5.015−04	6.466−04	2.485−03	6.245+00	3.633−03	1.338−01	1.653−04
.3673+02	1000.00	2.384−04	3.449−04	1.593−03	8.129+00	2.176−03	1.308−01	1.857−03
.4407+02	1200.00	1.165−04	1.848−04	1.004−03	1.020+01	1.305−03	1.138−01	2.399−03
.5509+02	1500.00	4.132−05	7.343−05	4.916−04	1.368+01	6.064−04	1.002−01	9.887−04
.7346+02	2000.00	7.820−06	1.599−05	1.433−04	2.037+01	1.671−04	1.006−01	−2.567−03
.9182+02	2500.00	1.557−06	3.536−06	4.042−05	2.823+01	4.551−05	1.007−01	−2.140−03
.1102+03	3000.00	3.296−07	7.903−07	1.118−05	3.733+01	1.229−05	1.244−01	1.954−03
.1469+03	4000.00	1.451−08	4.046−08	8.211−07	5.939+01	8.761−07	1.481−01	3.143−03
.1807+03	4920.00	8.839−10	2.678−09	7.140−08	8.380+01	7.496−08	2.021−01	−1.130−02
.1939+03	5280.00	2.985−10	9.293−10	2.726−08	9.443+01	2.848−08	2.465−01	−1.634−02
.2327+03	6336.00	1.263−11	4.205−11	1.596−09	1.297+02	1.651−09	5.964−01	−6.166−04
.2909+03	7920.00	1.152−13	4.134−13	2.197−11	1.943+02	2.250−11	1.415+00	1.177−01
.3394+03	9240.00	2.365−15	8.910−15	5.840−13	2.507+02	5.953−13	3.300+00	2.583−01

The good quality of the results shown in tables 4 and 5 is due largely to the predominance of the exponential trend of the unscattered photons throughout all scattered components. The approximations would not be satisfactory otherwise.

One should be aware that the error limits presented in tables 4 and 5 only pertain to one type of error. They do not include errors due to round-off in the calculation of moments, errors due to the finite numerical integration mesh in the calculation of moments or in the quadrature over the once-scattered components. And they take no cognizance of limits to the accuracy of the assumed interaction cross sections.

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A Theorem on Matrix Commutators

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Let $P=I_p \dot{+} (-I_q)$, the direct sum of the $p\times p$ identity matrix and the negative of the $q\times q$ identity matrix. The following theorem is proved.

THEOREM: *If the matrices* A *and* B *are* P*-orthogonal (orthogonal with respect to* P*) and* P*-skew-symmetric (skew-symmetric with respect to* P*) then* [A, B] = AB − BA *may be expressed as the difference,* C − D, *of matrices which are* P*-orthogonal,* P*-skew-symmetric.*

Explicit expressions for the matrices C and D are given.

Key words: Commutator; matrix; orthogonal; skew-symmetric.

1. Introduction

Let $P=I_p \dot{+} (-I_q)$, the direct sum of the $p\times p$ identity matrix and the negative of the $q\times q$ identity matrix. Katz and Olkin [1][2] define a matrix A to be orthogonal with respect to P (P-orthogonal) if only if

$$APA'=P \tag{1}$$

where A' is the transpose of the matrix A. Furthermore, they define a matrix B to be skew-symmetric with respect to P (P-skew-symmetric) if and only if the matrix BP is skew-symmetric in the ordinary sense.

The results of this paper are concerned with matrices which are both P-orthogonal and P-skew-symmetric of order $n=p+q$. J. M. Smith [4] proves that such matrices exist if and only if both n and p are even. Consider the following:

THEOREM 1: *If the* n × n *matrices* A *and* B *are both* P*-orthogonal and* P*-skew-symmetric then* [A, B] ≡ AB − BA *is a scaler multiple of a* P*-orthogonal,* P*-skew-symmetric matrix.*

The theorem has been proved in the cases $n=p=4$ and $n=p=2$ by Pearl [2] and in the case $n=4$, $p=2$ by J. M. Smith [3]. However, the above theorem is not true for all values of n and p. For example, let $n=p=6$ and let:

$$A=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad B=\begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}.$$

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[2] Figures in brackets indicate the literature references at the end of this paper.

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Thus Theorem 1 is not true without restrictions being placed on n and p.

In this paper, the following general theorem is proved:

THEOREM 2: *If* A *and* B *are both* P*-orthogonal,* P*-skew-symmetric matrices then*

$$[\mathrm{A}, \mathrm{B}] \equiv \mathrm{AB} - \mathrm{BA} = \mathrm{C} - \mathrm{D}$$

where C *and* D *are both* P*-orthogonal,* P*-skew-symmetric matrices.*

Theorem 2 is true for all values of n and p. Furthermore, explicit solutions are given for C and D in terms of A and B.

2. Proof of Theorem 2

Before proceeding, it is convenient to note the following:

LEMMA: *If the matrix* A *is* P*-skew-symmetric, then* $\mathrm{A}' = -\mathrm{PAP}$.

PROOF: Since A is P-skew-symmetric, AP is skew-symmetric and thus, $(AP)' = -AP$ or $P'A' = -AP$. But $P' = P$ and $P^2 = I$. Hence, $A' = -PAP$.

In order to prove Theorem 2, consider writing $[A, B]$ as $[A, B] = (AB + X) - (BA + X)$. The investigation of requisite properties of the matrix X in order that $AB + X$ and $BA + X$ be both P-orthogonal and P-skew-symmetric leads to the following result.

THEOREM 3: *Let* A *and* B *be* P*-orthogonal,* P*-skew-symmetric matrices. Then* $\mathrm{AB} + \mathrm{X}$ *and* $\mathrm{BA} + \mathrm{X}$ *are* P*-orthogonal,* P*-skew-symmetric matrices if and only if all of the following hold:*

(a)
$$\begin{aligned} \mathrm{XPX}' &= -(\mathrm{ABPX}' + \mathrm{XPB}'\mathrm{A}') \\ &= -(\mathrm{BAPX}' + \mathrm{XPA}'\mathrm{B}') \end{aligned}$$

(b)
$$\mathrm{X} + \mathrm{PX}'\mathrm{P} = -\mathrm{AB} - \mathrm{BA}$$

(c)
$$\mathrm{X}^2 = -\mathrm{P}(\mathrm{X}^2)'\mathrm{P}.$$

PROOF: Assume $AB + X$ and $BA + X$ to be P-orthogonal, P-skew-symmetric matrices. Since $AB + X$ is P-orthogonal,

$$(AB + X)\, P\, (AB + X)' = P$$

or
$$ABPB'A' + ABPX' + XPB'A' + XPX' = P$$

and by (1), $ABPB'A' = P$.

Hence,
$$ABPX' + XPB'A' + XPX' = 0. \tag{2}$$

Similarly since $BA + X$ is P-orthogonal

$$BAPX' + XPA'B' + XPX' = 0. \tag{3}$$

Equations (2) and (3) form condition (a). Furthermore, since $AB + X$ is P-skew-symmetric,

$$((AB + X)P)' = -(AB + X)P$$

or
$$P'B'A' + P'X' = -ABP - XP. \tag{4}$$

by the Lemma, $A' = -PAP$ and $B' = -PBP$ and since $P^2 = I$, (4) becomes

$$BAP + PX' = -ABP - XP.$$

Multiplying on the right by P,

$$BA+PX'P=-AB-X$$

which is condition (b). Similarly, the fact that $BA+X$ is P-skew-symmetric leads to condition (b). Finally, adding (2) and (3) one obtains

$$2XPX'+(AB+BA)\,PX'+XP\,(A'B'+B'A')=0$$

and applying condition (b) to the factors $AB+BA$ and $A'B'+B'A'$; gives condition (c).

Conversely, let a matrix X satisfy conditions (a), (b) and (c). By (c)

$$-X^2P-PX^{2\prime}=0$$

so that
$$2XPX'-XPX'-PX'^2-XPX'-X^2P=0$$

or
$$2XPX'+(-X-PX'P)\,PX'+XP\,(-X'-PXP)=0. \tag{5}$$

Applying condition (b) to (5),

$$2XPX'+(AB+BA)\,PX'+XP\,(A'B'+B'A')=0$$

or
$$(XPX'+ABPX'+XPB'A')+(XPX'+XPA'B'+BAPX')=0.$$

By condition (a) both of these terms are individually equal to zero. Thus it follows that $AB+X$ and $BA+X$ are P-orthogonal. Similarly, reversing the steps which led to condition (b), it follows that $AB+X$ and $BA+X$ are P-skew-symmetric.

It follows from Theorem 3 that if such a matrix X can be found the proof of Theorem 2 is completed. Letting $Y=XP$, then $Y'=PX'$ and multiplying (b) on the right by P

$$Y+Y'=-ABP-BAP.$$

Furthermore Y has a unique representation as the sum $S+Q$ of a symmetric matrix S and a skew-symmetric matrix Q. This leads to

COROLLARY 1: *The symmetric part of* Y *is uniquely given by*

$$\mathrm{S}=-\tfrac{1}{2}(\mathrm{AB}+\mathrm{BA})\,\mathrm{P}.$$

The skew-symmetric part of Y, Q, is not as easily found, however, certain conditions may be noted.

From (b) it follows that

$$X'=-PXP-PABP-PBAP$$

and substituting in both parts of (a) for X' leads to

$$XP(-PXP-PABP-PBAP)=ABXP+ABABP+ABBAP-XPB'A'$$

and

$$XP(-PXP-PABP-PBAP)=BAXP+BAABP+BABAP-XPA'B'.$$

Equating the expressions on the right and grouping appropriately leads to

$$[A,B]XP+XP[A',B']=BAABP-ABBAP+(BA)^2P-(AB)^2P.$$

Again, letting $Y=XP$ and noting that $A^2=-I$ and $B^2=-I$,

$$[A, B]Y-Y[A', B']=(BA)^2P-(AB)^2P.$$

Writing Y as $S+Q$, applying the fact that $A'B'=PABP$, and simplifying leads to

$$[A, B]Q+Q[A', B']=0.$$

Furthermore, by (c) $X^2=-P(X^2)'P$ and since $Y=XP$ then $YP=X$ or

$$(YP)^2=-P(YP)^2'P.$$

But $YP=SP+QP$ and hence

$$(SP)^2+(QP)^2+SPQP+QPSP=-(SP)^2-(QP)^2+QPSP+SPQP$$

or

$$(QP)^2=-(SP)^2.$$

Thus, by Corollary 1,

$$(QP)^2=-\tfrac{1}{4}(ABAB+BABA+2I).$$

This may be summarized as:

COROLLARY 2: *The skew-symmetric part* Q *of the matrix* Y *must satisfy both of the following conditions:*

(a) $$[\mathrm{A}, \mathrm{B}]\mathrm{Q}+\mathrm{Q}[\mathrm{A}', \mathrm{B}']=0$$

(b) $$(\mathrm{QP})^2=-\tfrac{1}{4}(\mathrm{ABAB}+\mathrm{BABA}+2\mathrm{I}).$$

While this does not uniquely define the matrix Q, it can be easily shown that one solution is

$$Q=\tfrac{1}{2}(ABABA+A)P.$$

Since $Y=S+Q$ and $X=YP$ it follows that the matrix

$$X=\tfrac{1}{2}(-AB-BA+ABABA+A)$$

satisfies all three conditions of Theorem 3.

Since $AB+X=\frac{1}{2}(AB-BA+ABABA+A)$ and $BA+X=\frac{1}{2}(-AB+BA+ABABA+A)$, Theorem 2 may be restated as a corollary of Theorem 3.

COROLLARY 3: Let A and B be P-orthogonal, P-skew-symmetric matrices. Then $[A, B]=C-D$ where C and D are P-orthogonal, P-skew-symmetric matrices. Furthermore,

$$C=\tfrac{1}{2}(AB-BA+ABABA+A),$$
$$D=\tfrac{1}{2}(-AB+BA+ABABA+A).$$

It should be noted that a second expression of the matrices C and D is obtained by interchanging A and B in the explicit expression given for C and D in the Corollary 3.

3. Conclusion

The main result of this paper, Theorem 2, may be stated as: Given any two P-orthogonal, P-skew-symmetric matrices A and B their commutator, $[A, B]$, may always be expressed as a linear combination (difference) of two other such matrices. Also, Corollary 3 gives an explicit representation of this linear combination.

An open question remains with regard to the matrix X defined in Theorem 3. Corollary 1 shows that the symmetric part of XP is unique. However, the skew-symmetric part of XP is not unique, and two expressions have been noted. Do other expressions exist and how may they be characterized?

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A Special Permutation Matrix Decomposition for Combinatorial Design Incidence Matrices*

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By a well-known theorem of König, every 0,1 matrix A of order v with all row and column sums equal to $k>0$ can be decomposed into a sum of k permutation matrices of order v. Here we consider whether A, trace $A=0$ or v, can have a special permutation matrix decomposition called a *special König decomposition*. The question is answered more or less satisfactorily using certain graph factorization theorems of Petersen and Tutte. Symmetric counterexamples are given to show that not all such matrices have special König decompositions; however, it is shown that symmetric incidence matrices *for* $\langle v, k, \lambda\rangle$ designs always have special König decompositions.

Key words: Block design; combinatorial analysis; configurations; König's theorem; matrices; 0,1 matrices; matrix equations; permutation matrix decompositions.

1. Introduction

A $\langle v, k\rangle$ *system* $[S, \mathscr{S}]$ is a set of v distinct elements $S=\{x_1, x_2, \ldots, x_v\}$ together with a selection of v not necessarily distinct subsets of S, $\mathscr{S}=\{X_1, X_2, \ldots, X_v\}$ such that each X_j contains exactly k of the elements in S and each x_i appears in exactly k of the subsets in S, $0\leq k\leq v$. If, in addition, we have $|X_1\cap X_j|=\lambda$ for each X_j, where $0<\lambda<k<v-1$, then we call $[S, \mathscr{S}]$ a $\langle v, k, \lambda\rangle$ *principal block partial design*, where X_1 is the *principal block*. If, further, we have $|X_i\cap X_j|=\lambda$ for every pair X_i, X_j, $i\neq j$, where $0<\lambda<k<v-1$, then $[S, \mathscr{S}]$ is known as a $\langle v, k, \lambda\rangle$ *design*. When $[S, \mathscr{S}]$ is a $\langle v, k, \lambda\rangle$ principal block partial design then, by a simple counting argument, we have:

$$(v-1)\lambda=k(k-1). \tag{1.1}$$

The incidence matrix of a $\langle v, k\rangle$ system $[S, \mathscr{S}]$ is the 0,1 matrix $A=[a_{ij}]$ of order v where:

$$a_{ij}=\begin{cases}1, & x_j\in S_i\\ 0, & x_j\notin S_i.\end{cases} \tag{1.2}$$

Note that each row and column sum of A is k. We denote the set of all such 0, 1 matrices by $\mathfrak{A}_v(k)$. Without loss of generality, we assume that the elements in S and the sets in $\mathscr{S}$ are ordered so that either $x_i\notin X_i$ for all $i=1, 2, \ldots, v$, or $x_i\in X_i$ for all $i=1, 2, \ldots, v$. Then we have either $\operatorname{tr} A=0$ or $\operatorname{tr} A=v$, respectively. Now, by a well-known theorem of König [3; p. 239, B.], A can be written as the sum of k permutation matrices of order v:

$$A=\delta I+\sum_{s=1}^{k-\delta}P_{r_s}, \qquad \delta=\begin{cases}0, & \operatorname{tr} A=0\\ 1, & \operatorname{tr} A=v\end{cases}, \tag{1.3}$$

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where P_{r_s} is the permutation matrix whose 1 in row 1 is in column r_s. We call (1.3) a *König decomposition of A*. If $B = [b_{ij}]$ and $c = [c_{ij}]$ are two 0, 1 matrices of order v, we write $B \cap C \equiv E$ for the matrix $E = [e_{ij}]$ of order v where $e_{ij} = \min\{b_{ij}, c_{ij}\}$, $i, j = 1, 2, \ldots, v$. We say that A *contains* the permutation matrix P or that P is *contained* in A if $A \cap P = P$.

In recent investigations on the above combinatorial designs [2] the authors encountered the following rather interesting problem. Let A be the incidence matrix of a $\langle v, k\rangle$ system. When is it possible to find a König decomposition (1.3) of A such that for each P_{r_s} in the decomposition either $P_{r_s}^T \cap A = 0$ or $P_{r_s}^T \cap A = P_{r_t}$ for some P_{r_t} in the decomposition? We call such a decomposition a *special König decomposition* of A. (If $A = 0$ or $A = I$ then A is considered to vacuously have a special König decomposition.) When $P_{r_s}^T \cap A = 0$, $P_{r_s} = [p_{ij}]$ has the properties that tr $P_{r_s} = 0$ and for no i, j, $i \neq j$, does $p_{ij} = p_{ji} = 1$. We call such a permutation matrix *skew*. When $P_{r_s}^T \cap A = P_{r_t}$ for some P_{r_t} then $P_{r_t} = P_{r_s}^T$ and either P_{r_s} is skew or else $P_{r_s}^T = P_{r_t} = P_{r_s}$ and P_{r_s} is a symmetric permutation matrix with tr $P_{r_s} = 0$. In the latter case we call P_{r_s} a 0-*symmetric* permutation matrix. Thus, a special König decomposition of A has the form

$$A = \delta I + \sum_{\alpha} P_{r_\alpha} + \sum_{\beta} (P_{r_\beta} + P_{r_\beta}^T) + \sum_{\gamma} P_{r_\gamma}, \tag{1.4}$$

where the P_{r_α}'s are the skew permutation matrices whose transposes do not occur in the decomposition, the P_{r_β}'s are the skew permutation matrices whose transposes do occur in the decomposition, and the P_{r_γ}'s are the 0-symmetric permutation matrices in the decomposition.

The following brief remarks are intended to convey the interest in the special König decomposition. In [2] the authors show that every abstract $\langle v, k\rangle$ system $[S, \mathscr{S}]$ can be isomorphically identified with a $\langle v, k\rangle$ system in an additive loop $\mathscr{L}$ of order v. In this identification, the elements of $[S, \mathscr{S}]$ correspond to the elements of $\mathscr{L}$ and the sets of $[S, \mathscr{S}]$ correspond to the left translates $l + D$, $l \in \mathscr{L}$, of a k-subset D of $\mathscr{L}$. The identification is obtained via König decompositions of the incidence matrices A of $[S, \mathscr{S}]$ and A_c of the complementary system $[S, \mathscr{S}_c]$, $\mathscr{S}_c = \{\mathscr{S} - X_1, \ldots, S - X_v\}$. Under this identification, the set of elements D is right inversive in $\mathscr{L}$ if and only if A has a special König decomposition, and $\mathscr{L}$ is a right inverse property loop if and only if both A and A_c have special König decompositions. When D is right inversive, D forms a difference set in $\mathscr{L}$ if and only if $[S, \mathscr{S}]$ is a $\langle v, k, \lambda\rangle$ principal block partial design. This situation has further combinatorial implications, which can be found in [2].

Since not all $\langle v, k\rangle$ system incidence matrices A, with tr $A = 0$ or tr $A = v$, have a special König decomposition, we need to find conditions on A such that A does have such a decomposition. Let us suppose that A has a special König decomposition. We consider a pair a_{ij}, a_{ji}, $i \neq j$, where $a_{ij} = a_{ji} = 1$. This pair of 1's must either be entries in a 0-symmetric permutation matrix P_{r_γ} or of a transpose-pair of skew permutation matrices P_{r_β}, $P_{r_\beta}^T$. All such pairs of 1's appear in the matrix $A_s \equiv A \cap A^T$. Note that $A_q \equiv A - A_s = [a_{ij}^{(q)}]$ has the property that if $a_{ij}^{(q)} = 1$, $i \neq j$, then $a_{ji}^{(q)} = 0$. Thus, a necessary condition for A to have a special König decomposition is that $A_s \in \mathfrak{A}_v(k_s)$ (whence $A_q \in \mathfrak{A}_v(k - k_s)$) for some k_s, $0 \leq k_s \leq k$. Now, a special König decomposition of A induces special König decompositions of A_s and A_q, and conversely. Since $A \cap A_q^T = 0$, it is easy to see that every König decomposition of A_q is a special König decomposition. Thus, we can reduce the problem to symmetric matrices:

LEMMA 1.1: *Let* $\mathrm{A} \in \mathfrak{A}_\mathrm{v}(\mathrm{k})$, *where* tr $\mathrm{A} = 0$ *or* tr $\mathrm{A} = \mathrm{v}$. *Then necessary and sufficient conditions for* A *to have a special König decomposition are that*

(a) $\mathrm{A_s} \in \mathfrak{A}_\mathrm{v}(\mathrm{k_s})$ *for some* $\mathrm{k_s}$, $0 \leq \mathrm{k_s} \leq \mathrm{k}$, *and*

(b) $\mathrm{A_s}$ *have a special König decomposition.*

For any given A, condition (a) is easy to decide. So we invoke this reduction and assume that A is symmetric, i.e., $A = A_s$, $k = k_s$, and $A_q = 0$. Here (1.4) becomes:

$$A = \delta I + \sum_{\beta} (P_{r_\beta} + P_{r_\beta}^T) + \sum_{\gamma} P_{r_\gamma}. \tag{1.5}$$

We shall call A 0-*symmetric* or *co-symmetric* according as tr $A=0$ or tr $A=v$. We note that if A contains a 0-symmetric permutation matrix then v must be even.

In this paper we settle more or less satisfactorily the question of whether a 0-symmetric or co-symmetric A has a special König decomposition by first transforming the question into a natural problem on regular graphs and then applying two theorems in graph theory concerning the existence of 1-factors and 2-factors in such graphs. For the cases where only 2-factors need be considered, the matrix A always has a special König decomposition by a theorem of Petersen. For the cases where 1-factors must be considered, the question is not as satisfactorily answered since the answer is determined by the criterion in Tutte's theorem on the existence of 1-factors in a graph, and it is not easy, in general, to apply this criterion. In this regard, we show that in such cases A need not have a special König decomposition. In fact, we exhibit 0-symmetric and co-symmetric A's which are incidence matrices for $\langle v, k, \lambda\rangle$ principal block partial designs which do not have special König decompositions. Finally, however, we do show, using a corollary of Tutte's theorem for regular graphs, that in all cases where A is the incidence matrix for a $\langle v, k, \lambda\rangle$ design, A always has a special König decomposition.

2. Main Results

Again, let A be a 0-symmetric or co-symmetric 0, 1 matrix in $\mathfrak{A}_v(k)$, $0 \leq k \leq v$. We define

$$\hat{A}=\begin{cases} A, \text{tr}\, A=0 \\ A-I, \text{tr}\, A=v. \end{cases}$$

Then $\hat{A}$ will be interpreted as the adjacency matrix of a regular graph $\mathcal{G}(V, \hat{k})$ of degree $\hat{k}$ on v vertices $V=\{v_1, \ldots, v_v\}$, in this order, where

$$\hat{k}=\begin{cases} k, \text{tr}\, A=0 \\ k-1, \text{tr}\, A=v. \end{cases}$$

An *m-factor* of $\mathcal{G}(V, \hat{k})$ is a subgraph $\mathcal{G}(V, m)$ of degree $m>0$ on the full set of vertices V, and we say that $\mathcal{G}(V, \hat{k})$ is *factorable* into regular factors $\mathcal{G}(V, m_i)$, $i=1, 2, \ldots, t$, if

$$\mathcal{G}(V, \hat{k})=\sum_{i=1}^{t} \mathcal{G}(V, m_i),$$

where the summation indicates that the set of edges in $\mathcal{G}(V, \hat{k})$ is the union of the sets of edges in the factors $\mathcal{G}(V, m_i)$. (For $t=0$ this is the vacuous factorization for either $A=0$ or $A=I$.) We note that the adjacency matrix of a 1-factor of $\mathcal{G}(V, \hat{k})$ is a 0-symmetric permutation matrix contained in A, and that the adjacency matrix of a 2-factor of $\mathcal{G}(V, \hat{k})$ is the sum of a skew permutation matrix and its transpose, both of which are contained in A. Hence, by (1.5) we have:

LEMMA 2.1: A *has a special König decomposition if and only if* $\mathcal{G}(V, \hat{k})$ *is factorable into regular factors of degrees* 1 *and* 2.

We first note that when v is odd and $\hat{k}$ is odd Lemma 2.1 requires that $\mathcal{G}(V, \hat{k})$ have a 1-factor, which means that v must be even, a contradiction. Actually, A does not even exist in this case, since here the total sum of vertex degrees in $\mathcal{G}(V, \hat{k})$ would be $v\hat{k}$, which is odd, but would also be twice the number of edges in $\mathcal{G}(V, \hat{k})$, which is even, a contradiction. Thus,

THEOREM 2.2: A *does not exist for* v *odd when*

(i) k *is odd and* tr A$=0$.
(ii) k *is even and* tr A$=v$.

Now, relevant to our investigation here for other cases is the following result due to Petersen [4]:

THEOREM 2.3. *A regular graph of even degree* d = 2e *is factorable into* e *2-factors.*

By this theorem we then have

THEOREM 2.4: A *has a special König decomposition when*

(i) k *is even and* tr A = 0.
(ii) k *is odd and* tr A = v.

By Theorems 2.2 and 2.4 the remaining undecided cases are for v even with either k odd and tr $A=0$ or k even and tr $A=v$. In these cases the graph $\mathcal{G}(V, \hat{k})$ has $\hat{k}$ odd. Thus, if A is to have a special König decomposition here, $\mathcal{G}(V, \hat{k})$ must have a 1-factor. Further, this condition is sufficient since then the subgraph of $\mathcal{G}(V, \hat{k})$ remaining after removal of a 1-factor would be regular of even degree $\hat{k}-1$, which, by Theorem 2.3, would factor into $(\hat{k}-1)/2$ 2-factors. Relevant to our investigation here is the following result due to Tutte [5]:

THEOREM 2.5: *Let* $\mathcal{G}$ *be a connected graph on a set of vertices* X. *For any proper subset* Y *of* X *let* θ(Y) *denote the number of components of odd order in the subgraph of* $\mathcal{G}$ *determined by the vertices* X − Y. *Then, a necessary and sufficient condition for* $\mathcal{G}$ *to have a 1-factor is that* $\theta(Y) \leq |Y|$ *for every proper subset* Y *of* X.

Applying this theorem to the 0-symmetric or co-symmetric matrix A we have:

THEOREM 2.6: A *has a special König decomposition when*

(i) k *is odd and* tr A = 0, *or*
(ii) k *is even and* tr A = v,

if and only if for every irreducible direct summand A′ *of* A, A′ *is of even order and the necessary and sufficient condition of Theorem* 2.5 *holds for the component of* $\mathcal{G}(V, \hat{k})$ *whose adjacency matrix is* A′.

We apply Theorem 2.5 to show that in these two undecided cases A need not have a special König decomposition. In fact, our counterexamples will be 0-symmetric and co-symmetric incidence matrices for $\langle v, k, \lambda \rangle$ principal block partial designs.

Counterexample 1. v even, k odd, tr $A=0$: $v=106$, $k=15$, $\lambda=2$.

Let $\bar{e}=[1\ 1\ 1\ 1\ 1]$, $\bar{0}=[0\ 0\ 0\ 0\ 0]$, and form $\bar{u}=[\bar{e}, \bar{0}, \bar{0}, \bar{0}, \bar{0}, \bar{0}]$ of length 35.

Let

$$B=\begin{bmatrix} 0&1&1&0&0\\ 1&0&0&1&0\\ 1&0&0&0&1\\ 0&1&0&0&1\\ 0&0&1&1&0 \end{bmatrix}, \quad C=\begin{bmatrix} 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{bmatrix}, \quad D=\begin{bmatrix} 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{bmatrix}, \quad E=\begin{bmatrix} 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0 \end{bmatrix},$$

$$F=\begin{bmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1 \end{bmatrix}, \quad G=\begin{bmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1 \end{bmatrix}, \quad H=\begin{bmatrix} 0&1&1&1&1&1\\ 1&0&1&1&1&1\\ 1&1&0&1&1&1\\ 1&1&1&0&1&1\\ 1&1&1&1&0&1\\ 1&1&1&1&1&0 \end{bmatrix}, \quad K=\begin{bmatrix} 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 1&1&1&1&1&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{bmatrix},$$

$$L=\begin{bmatrix}1&1&0&0&0&0\\0&0&1&1&1&1\\0&0&0&0&0&0\\1&1&0&0&0&0\\0&0&1&1&1&1\\0&0&0&0&0&0\end{bmatrix},\quad M=\begin{bmatrix}0&0&0&0&0&0\\1&1&1&1&0&0\\0&0&0&0&1&1\\0&0&0&0&0&0\\1&1&1&1&0&0\\0&0&0&0&1&1\end{bmatrix},\quad N=\begin{bmatrix}0&0&0&0&0&0\\0&0&0&0&0&0\\1&1&1&1&1&1\\0&0&0&0&0&0\\0&0&0&0&0&0\\1&1&1&1&1&1\end{bmatrix},\quad Q=\begin{bmatrix}0&0&0&0&0&0\\1&1&1&1&1&1\\0&0&0&0&0&0\\0&0&0&0&0&0\\1&1&1&1&1&1\\0&0&0&0&0&0\end{bmatrix},$$

$$R=\begin{bmatrix}1&1&1&1&0&0\\0&0&0&0&1&1\\0&0&0&0&0&0\\1&1&1&1&0&0\\0&0&0&0&1&1\\0&0&0&0&0&0\end{bmatrix},\quad S=\begin{bmatrix}0&0&0&0&0&0\\1&1&0&0&0&0\\0&0&1&1&1&1\\0&0&0&0&0&0\\1&1&0&0&0&0\\0&0&1&1&1&1\end{bmatrix},\quad T=\begin{bmatrix}1&1&0&0&0&0\\0&0&1&1&0&0\\0&0&0&0&1&1\\1&1&0&0&0&0\\0&0&1&1&0&0\\0&0&0&0&1&1\end{bmatrix},$$

and form

$$U=\begin{bmatrix}B&C&D&E&F&G\\C^T&H&K&L&M&N\\D^T&K^T&H&K&Q&N\\E^T&L^T&K^T&H&R&S\\F^T&M^T&Q^T&R^T&H&T\\G^T&N^T&N^T&S^T&T^T&H\end{bmatrix}$$

of order 35. Let $\mathbf{0}$ denote the zero matrix of order 35. Finally, form

$$\mathrm{A}_{106}=\begin{bmatrix}0&\bar{u}&\bar{u}&\bar{u}\\\bar{u}^T&U&\mathbf{0}&\mathbf{0}\\\bar{u}^T&\mathbf{0}&U&\mathbf{0}\\\bar{u}^T&\mathbf{0}&\mathbf{0}&U\end{bmatrix}$$

of order 106 with row sums and column sums all equal to 15 and all inner products of row 1 with any other row equal to 2. Let $\mathscr{G}_{106}$ be the connected graph of degree 15 on the 106 vertices $V=\{v_1, v_2, \ldots, v_{106}\}$ whose adjacency matrix is A_{106}. For $\mathrm{Y}=\{v_1\}$, $\theta(Y)=3>1=|Y|$, hence, by Theorem 2.5, $\mathscr{G}_{106}$ does not have a 1-factor, whence A_{106} does not have a special König decomposition.

Counterexample 2. v even, k even, $\mathrm{tr}\,A=v: v=46$, $k=10$, $\lambda=2$.

Let $\bar{e}=[1\ 1\ 1]$, $\bar{0}=[0\ 0\ 0\ 0]$ and form $\bar{w}=[\bar{e}, \bar{0}, \bar{0}, \bar{0}]$ of length 15.

Let

$$I_3=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix},\ B=\begin{bmatrix}1&1&1&1\\1&1&1&1\\0&0&0&0\end{bmatrix},\ C=\begin{bmatrix}1&1&1&1\\0&0&0&0\\1&1&1&1\end{bmatrix},\ D=\begin{bmatrix}0&0&0&0\\1&1&1&1\\1&1&1&1\end{bmatrix},$$

$$J_4=\begin{bmatrix}1&1&1&1\\1&1&1&1\\1&1&1&1\\1&1&1&1\end{bmatrix},\ E=\begin{bmatrix}1&1&1&1\\0&0&0&0\\1&1&1&1\\0&0&0&0\end{bmatrix},\ F=\begin{bmatrix}0&0&0&0\\1&1&1&1\\0&0&0&0\\1&1&1&1\end{bmatrix},\ G=\begin{bmatrix}1&1&0&0\\0&0&1&1\\1&1&0&0\\0&0&1&1\end{bmatrix},$$

and form

$$W=\begin{bmatrix}I_3&B&C&D\\B^T&J_4&E&F\\C^T&E^T&J_4&G\\D^T&F^T&G^T&J_4\end{bmatrix}$$

of order 15. Let $\mathbf{0}$ denote the zero matrix of order 15. Finally, form

$$A_{46}=\begin{bmatrix} 1 & \bar{w} & \bar{w} & \bar{w} \\ \bar{w}^T & W & \mathbf{0} & \mathbf{0} \\ \bar{w}^T & \mathbf{0} & W & \mathbf{0} \\ \bar{w}^T & \mathbf{0} & \mathbf{0} & W \end{bmatrix}$$

of order 46 with row sums and column sums all equal to 10 and all inner products of row 1 with any other row equal to 2. Let $\mathcal{G}_{46}$ be the connected graph of degree 9 on the 46 vertices $V=\{v_1, v_2, \ldots, v_{46}\}$ whose adjacency matrix is $A_{46}-I$. For $Y=\{v_1\}$, $\theta(Y)=3>1=|Y|$, hence, by Theorem 2.5, $\mathcal{G}_{46}$ does not have a 1-factor, whence A_{46} does not have a special König decomposition.

We now show that a 0-symmetric or co-symmetric incidence matrix for a $\langle v, k, \lambda\rangle$ design does have a special König decomposition. Relevant to the proof of this result is the following corollary to Theorem 2.5 [1; p. 182, Theorem 6].

COROLLARY 2.7. *Let $\mathcal{G}$ be a connected regular graph of degree* h *on a set* X *of an even number of vertices. For any proper subset* Y *of* X *let* η(Y) *denote the number of edges in $\mathcal{G}$ which connect a vertex in* Y *with a vertex in* X$-$Y. *Then a sufficient condition for $\mathcal{G}$ to have a* 1*-factor is that* $\eta(Y)\geq h-1$ *for every proper subset* Y *of* X.

We note that the sufficient condition in this corollary is not a necessary condition, as is easily seen in the following graph of degree 3 on 10 vertices:

Now, the theorem for $\langle v, k, \lambda\rangle$ designs.

THEOREM 2.8. *Let* A *be a 0-symmetric or co-symmetric incidence matrix for a* $\langle$v, k, $\lambda\rangle$ *design. Then* A *has a special König decomposition.*

PROOF: By Theorems 2.2 and 2.4 we may limit our attention to the cases for v even where either k is odd and tr $A=0$ or k is even and tr $A=v$. We choose any proper subset of μ rows of A and we permute the rows of A such that these μ rows become the first μ rows. We perform this same permutation on the columns of the resulting matrix. We then obtain a 0-symmetric or co-symmetric matrix of the form

$$PAP^T=\begin{bmatrix} F & E \\ E^T & G \end{bmatrix}, \tag{2.1}$$

where P is the permutation matrix inducing the above permutation of the rows of A, F is of order μ, and G is of order $v-\mu$. Let e denote the number of 1's in E. Then the number of 1's in F is $\sigma=\mu k-e$, and the number of 1's in G is $\tau=(v-\mu)k-e$. Considering $\hat{A}$ as the adjacency matrix of a regular graph $\mathcal{G}(V, \hat{k})$ and Y as the set of μ vertices of $\mathcal{G}(V, \hat{k})$ given by the proper subset of μ rows and columns of $\hat{A}$, we see that $\eta(Y)=e$. Thus, since these μ vertices, $1\leq\mu\leq v-1$, are arbitrary, if we can show that

$$e\geq\hat{k}-1=\begin{cases} k-1, \text{ tr } A=0 \\ k-2, \text{ tr } A=v \end{cases}, \tag{2.2}$$

then, by Corollary 2.7 (since $e\geq k-2>0$ for any choice of μ vertices implies the graph is connected), we will have shown that $\mathcal{G}(V, \hat{k})$ has a 1-factor, which, by our previous discussion, implies that A has a special König decomposition. So, suppose that $e\leq k-2$. Then, since the number of entries in F is μ^2, we have

$$\mu^2\geq\sigma=\mu k-e\geq\mu k-k+2,$$

or

$$\left(\mu-\frac{k}{2}\right)^2 \geq \left(\frac{k}{2}\right)^2 - k + 2 > \left(\frac{k}{2}-1\right)^2,$$

or, since $k > 2$,

$$\left|\mu-\frac{k}{2}\right| > \frac{k}{2}-1. \tag{2.3}$$

Now, if $\mu < \frac{k}{2}$ then (2.3) would imply that $\mu < 1$, a contradiction. Hence, $\mu \geq \frac{k}{2}$ and from (2.3) we have

$$\mu \geq k. \tag{2.4}$$

By a similar argument, comparing the number of entries in G with τ, we obtain the corresponding result

$$\mu \leq v-k. \tag{2.5}$$

We now let σ_i denote the sum of column i in F, $1 \leq i \leq \mu$. Then, counting all inner products of ordered pairs of rows of F, we see, noting that all entries are 0 or 1, that

$$\sum_{i=1}^{\mu} \sigma_i^2 \leq \sigma + \mu(\mu-1)\lambda. \tag{2.6}$$

Now, by the theorem of the means,

$$\frac{1}{\mu}\sum_{i=1}^{\mu} \sigma_i^2 \geq \left(\frac{1}{\mu}\sum_{i=1}^{\mu} \sigma_i\right)^2 = \frac{\sigma^2}{\mu^2},$$

hence, by (2.6),

$$\sigma^2 - \mu\sigma \leq \mu^2(\mu-1)\lambda,$$

or

$$\left(\sigma-\frac{\mu}{2}\right)^2 \leq \left(\frac{\mu}{2}\right)^2 \{4(\mu-1)\lambda+1\},$$

whence, since $\sigma = \mu k - e$,

$$\left|\mu\left(k-\frac{1}{2}\right)-e\right| \leq \frac{\mu}{2}\sqrt{4(\mu-1)\lambda+1}. \tag{2.7}$$

Now, since $\mu \geq k > 2$, if $e \geq \mu(k-\frac{1}{2})$ then $e \geq \mu(k-\frac{1}{2}) > k-\frac{1}{2} > k-1$, which is contrary to our assumption that $e \leq k-2$. Hence $e < \mu(k-\frac{1}{2})$ and (2.7) becomes

$$e > \mu\{k-\tfrac{1}{2}-\tfrac{1}{2}\sqrt{4(\mu-1)\lambda+1}\}. \tag{2.8}$$

Then, by (2.4), (2.5), and (2.8) we have

$$e > k\{k-\tfrac{1}{2}-\tfrac{1}{2}\sqrt{4(v-k-1)\lambda+1}\}$$

which, since $(v-1)\lambda = k^2-k$, becomes

$$e > k\{k-\tfrac{1}{2}-\sqrt{(k-\tfrac{1}{2})^2-k\lambda}\ \}. \tag{2.9}$$

Now, since v is even and $(v-1)\lambda = k(k-1)$ is always even, we have λ even, implying $\lambda \geq 2$, whence $k(\lambda-2) \geq 0$, or

$$k^2-3k+(\tfrac{3}{2})^2 \geq k^2-k-k\lambda+(\tfrac{3}{2})^2,$$

or

$$(k-\tfrac{3}{2})^2 \geq (k-\tfrac{1}{2})^2-k\lambda+2 > (k-\tfrac{1}{2})^2-k\lambda > 0,$$

whence, since $k > 2$,

$$k-\tfrac{3}{2} > \sqrt{(k-\tfrac{1}{2})^2-k\lambda}. \tag{2.10}$$

Combining (2.9) and (2.10) yields

$$e > k\{k-\tfrac{1}{2}-k+\tfrac{3}{2}\} = k \tag{2.11}$$

which is also contrary to our assumption that $e \leq k-2$. Hence, $e \geq k-1$ and by (2.2) we have the theorem.

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The Casimir Check for the Algebraic Matrices of the Configuration $(d+s)^n p$*

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By using the eigenvalues of the Casimir operator for the group SU_3, checking parameters were obtained for 12 electrostatic interaction matrices of the configuration $(d+s)^n p$.

Key words: Casimir operator, checking parameters, $(d+s)^n p$, SU_3.

1. Introduction

The algebraic matrices of $(d+s)^n p$ comprise the electrostatic and spin-orbit interaction matrices of the configurations $d^n p$, $d^{n-1}sp$ and $d^{n-2}s^2 p$, the matrices of the correction parameters representing two and three body interactions of the core d electrons, as well as the matrices of the interactions between configurations. The energy matrix (for a particular n) is then a linear combination of these matrices, the coefficients of which are parameters usually obtained empirically by fitting the experimental levels to the eigenvalues of the energy matrix. The following lists these parameters and gives their significance. Unprimed quantities denote the configuration $d^n p$, primes denote $d^{n-1}sp$ and double primes $d^{n-2}s^2 p$.

A, A', A'', the heights of the configurations
$S' = A' - A$, $S'' = A'' - A$

B, B', B'' linear combinations of the Slater parameters $F^2(dd)$ and $F^4(dd)$

$$B = 1/441\ [9F^2(dd) - 5F^4(dd)] = F_2(dd) - 5F_4(dd) \quad [1][1]$$

C, C', C'' multiples of the Slater parameter $F^4(dd)$ [1]

$$C = 5/63\ F^4(dd) = 35\ F_4(dd)$$

G'_{ds} the parameter of the $d-s$ interaction in the configuration $d^{n-1}sp$

$$G'_{ds} = 1/5G^2(ds) \quad [2]$$

F_2, F'_2, F''_2 parameters of the direct part of the $d-p$ interaction

$$F_2 = 1/35F^2(dp) \quad [1]$$

G_1, G'_1, G''_1 parameters of the exchange part of the $d-p$ interaction

$$G_1 = 1/15G^1(dp) \quad [1]$$

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[1] Figures in brackets indicate the literature references at the end of this paper.

G_3, G_3', G_3'' parameters of the exchange part of the $d-p$ interaction

$$G_3 = 3/245 G^3(dp)$$

G'_{ps} the parameter of the $p-s$ interaction in the configuration $d^{n-1}sp$

$$G'_{ps} = 1/3 G^1(ps) \qquad [3, 8^6]$$

$\alpha, \alpha', \alpha''$ correction parameters multiplying $L_1(L_1+1)$, where L_1 is the angular momentum of the core of $(d+s)^n p$, i.e., $(d+s)^n$ [4–6]

β, β', β'' correction parameters multiplying the seniority operator of Racah [2, 7]

T, T', T'' parameters of Trees multiplying the squared matrix of the interaction

$$3s^2\, 3d^n - 3s\, 3d^{n+1} \qquad [8, 9]$$

H parameter of the $d^n - d^{n-1}s$ interaction

$$H = R^2(dd, ds)/35$$

H' parameter of the $d^{n-1}s - d^{n-2}s^2$ interaction, defined the same as H

J parameter of the direct part of the $d^n p - d^{n-1}sp$ interaction,

$$J = R^2(dp, sp)/5 \qquad [10, 11]$$

J' parameter of the direct part of the $d^{n-1}sp - d^{n-2}s^2p$ interaction defined the same as J.

K parameter of the exchange part of the $d^n p - d^{n-1}sp$ interaction,

$$K = R^1(dp, ps)/3 \qquad [10, 11]$$

K' parameter of the exchange part of the $d^{n-1}sp - d^{n-2}s^2p$ interaction defined the same as K.

G parameter of the $d^n p - d^{n-2}s^2p$ interaction

$$G = R^2(dd, ss)/5 = R^2(ds, sd)/5 = G^2(ds)/5 = G'_{ds} \qquad [2]$$

$\zeta_d, \zeta'_d, \zeta''_d$ parameters of the spin-orbit interaction of the d electrons [2]

$\zeta_p, \zeta'_p, \zeta''_p$ parameters of the spin-orbit interaction of the p electron [2]

$\lambda, \lambda', \lambda''$ checking parameters multiplying $L(L+1)$, where L is the net angular momentum for a particular term of $(d+s)^n p$

$\delta, \delta', \delta''$ checking parameters multiplying $S(S+1) - S_1(S_1+1)$, where S is the net spin of $(d+s)^n p$ and S_1 is the net spin of $(d+s)^n$.

The algebraic matrices of $(d+s)^n p$ were constructed and checked by the author with the purpose of using them to explain and predict the spectra of the configurations $(3d+4s)^n 4p$ in neutral and singly ionized atoms of the iron group. The problem of constructing the matrices was considered previously, [11–13]. The purpose of the present paper is to describe a principal check for the algebraic matrices. The checked matrices of the configurations $(d+s)^n p$, for all permissible n, are available and can be obtained by request.

All checks are based upon the construction of such combinations of algebraic matrices so that the eigenvalues of the resulting matrix may be predicted theoretically. If we know the values

of the parameters required in order to form the desired linear combinations, then we insert these values as coefficients multiplying the algebraic matrices found on tape, and diagonalize the resulting matrix. If the obtained eigenvalues differ from those predicted theoretically then it is usually not too difficult to find the reason for the discrepancy because in a particular check only a few of the algebraic matrices are utilized.

2. Predicted Eigenvalues and Their Multiplicities

As explained by Elliott [14] the eigenfunctions of a single particle which may be either in a d shell or an s shell can be considered as the basis of the representation (200) of the three dimensional unitary group U_3. The eigenfunctions of a system of n such particles may be classified according to the irreducible representations of U_3 which appear in the reduction of the nth power of the representation (200). The electron p can be considered as belonging to (100). We write these representations as (p, q, r) where p, q, r represent the lengths of the rows of the Young's tableau and $p \geq q \geq r$. For $(d+s)^n$, $p+q+r$ equals $2n$, whereas for $(d+s)^n p$, $p+q+r$ equals $2n+1$. The representations of U_3 which differ only by a number of columns of three blocks are equivalent representations of SU_3. Since R_3, whose representation is characterized by L is a subgroup of SU_3, we can always subtract r blocks from each row. The separation of the states belonging to the different representations may be made by an interaction whose eigenvalues are proportional to the Casimir operator of the group SU_3. If these eigenvalues are given by $g(p, q, r)$ we have the relationship

$$g(p, q, r) = g(p-r, q-r, 0) \tag{1}$$

Explicitly we have, [15]

$$g(p, q, r) = p^2 + q^2 + r^2 - pq - pr - qr + 3p - 3r. \tag{2}$$

The relationship (1) can also be checked directly from (2).

From Hamermesh [16], we obtain the rules of multiplying the Young's tableaux. From a paper by Racah [17] it is possible to obtain the values of L which appear in each tableau. Table 1 gives the values of L and the value of $2g$ for each particular tableau.

TABLE 1. *Values of* L *appearing in the representations of* SU_3

Representation	Values of L	2g	Representation	Values of L	2g
(00)	S	0	(52)	P D F F G H	68
(10)	P	8	(62)	S D D F G G H I	92
(20)	S D	20	(72)	P D F F G H H I K	120
(30)	P F	36	(33)	P F	36
(40)	S D G	56	(43)	P D F G	50
(50)	P F H	80	(53)	P D F F G H	68
(60)	S D G I	108	(63)	P D F F G G H I	90
(70)	P F H K	140	(73)	P D F F G G H H I K	116
(11)	P	8	(44)	S D G	56
(21)	P D	18	(54)	P D F G H	72
(31)	P D F	32	(64)	S D D F G G H I	92
(41)	P D F G	50	(74)	P D F F G G H H I K	116
(51)	P D F G H	72	(55)	P F H	80
(61)	P D F G H I	98	(65)	P D F G H I	98
(71)	P D F G H I K	128	(75)	P D F F G H H I K	120
(22)	S D	20	(66)	S D G I	108
(32)	P D F	32	(76)	P D F G H I K	128
(42)	S D D F G	48	(77)	P F H K	140

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In order to obtain the tableaux of $(d+s)^n$, we consider two groups of electrons. Let the first group be of $(d+s)^x$, with all the electrons having m_s equal to 1/2 and thus M_s equals $x/2$. Let the second group be of $(d+s)^{n-x}$ with all the electrons having m_s equal to $-1/2$ and thus M_s equals $-(n-x)/2$. In each group we use Pauli's principle by taking the tableau(x) of maximal spin. Between the two groups Pauli's principle does not apply since they have different m_s. By multiplying the tableaux we get all the terms of $(d+s)^n$, with M_s being equal to $(2x-n)/2$ and S taking on the values between $n/2$ and $|2x-n|/2$.

We now give the tableaux for $(d+s)^n$, and $(d+s)^n p$, where $n \leq 6$. The superscript on each tableau indicates the spin. Thus, the tableau of $(d+s)$ is written as $^2(200)$.

In order to obtain the tableaux of $(d+s)p$, it is necessary to multiply the above tableau by $^2(100)$. Then, $(d+s)p$ is given by

$$^2(200) \times {}^2(100) = {}^{1,3}(300) + {}^{1,3}(210)$$

For $(d+s)^2$ we have

$$(200) \times (200) = (400) + (220) + (310).$$

By Pauli's principle we don't get singlets and triplets for each tableau. However, by a comparison with the known terms of $(d+s)^2$, we can write

$$(d+s)^2\text{:} \quad {}^1(400) + {}^1(220) + {}^3(310).$$

To obtain $(d+s)^2 p$, we simply multiply the above by $^2(100)$. Then,

$$(d+s)^2 p\text{:} \quad {}^2(500) + {}^2(410) + {}^2(320) + {}^2(221) + {}^{2,4}(410) + {}^{2,4}(320) + {}^{2,4}(311).$$

The tableaux of $(d+s)^3$ are obtained by multiplying (310), which is the tableau of highest spin in $(d+s)^2$, by (200). Again by comparing with the known terms of $(d+s)^3$ we can write

$$\begin{aligned}(d+s)^3\text{:} \quad & {}^2(510) + {}^2(420) + {}^2(321) + {}^4(411) + {}^4(330) \\ (d+s)^3 p\text{:} \quad & {}^{1,3}(610) + {}^{1,3}(520) + {}^{1,3}(511) + {}^{1,3}(520) + {}^{1,3}(430) + {}^{1,3}(421) + {}^{1,3}(421) \\ & + {}^{1,3}(331) + {}^{1,3}(322) + {}^{3,5}(511) + {}^{3,5}(421) + {}^{3,5}(430) + {}^{3,5}(331).\end{aligned}$$

To obtain the tableaux of $(d+s)^4$ we multiply (310) by (310). We note that in order to get only the triplets and quintets of $(d+s)^4$, we can multiply $(411)+(330)$, which are of highest spin in $(d+s)^3$, by (200). The latter multiplication is useful in helping to identify the spins of the various tableaux obtained by the multiplication of (310) by (310), which gives all the spins. Then by comparing with the known terms of $(d+s)^4$, we have

$$\begin{aligned}(d+s)^4\text{:} \quad & {}^1(620) + {}^1(440) + {}^1(422) + {}^1(521) + {}^3(611) + {}^3(530) + {}^3(521) + {}^3(431) + {}^3(332) \\ & + {}^5(431)\end{aligned}$$

$$\begin{aligned}(d+s)^4 p\text{:} \quad & {}^2(720) + {}^2(630) + {}^2(621) + {}^2(540) + {}^2(441) + {}^2(522) + {}^2(432) + {}^2(621) \\ & + {}^2(531) + {}^2(522) + {}^{2,4}(711) + {}^{2,4}(621) + {}^{2,4}(630) + {}^{2,4}(540) + {}^{2,4}(531) \\ & + {}^{2,4}(621) + {}^{2,4}(531) + {}^{2,4}(522) + {}^{2,4}(531) + {}^{2,4}(441) + {}^{2,4}(432) + {}^{2,4}(432) \\ & + {}^{2,4}(333) + {}^{4,6}(531) + {}^{4,6}(441) + {}^{4,6}(432).\end{aligned}$$

To obtain the tableaux of $(d+s)^5$ we multiply (411)+(330), which are of spin 3/2 in $(d+s)^3$, by (310), which is of highest spin in $(d+s)^2$. Again, it is very useful to multiply (431), which is the tableau representing spin 2 in $(d+s)^4$, by (200). The latter result yields the quartets and sextets of $(d+s)^5$. By checking with the known terms of $(d+s)^5$ we have

$$
\begin{aligned}
(d+s)^5\text{:}\quad & {}^2(721)+{}^2(622)+{}^2(640)+{}^2(631)+{}^2(541)+{}^2(532)+{}^2(442)+{}^4(631)\\
& +{}^4(541)+{}^4(532)+{}^4(433)+{}^6(442)\\
(d+s)^5p\text{:}\quad & {}^{1,3}(821)+{}^{1,3}(731)+{}^{1,3}(722)+{}^{1,3}(722)+{}^{1,3}(632)+{}^{1,3}(740)+{}^{1,3}(650)\\
& +{}^{1,3}(641)+{}^{1,3}(731)+{}^{1,3}(641)+{}^{1,3}(632)+{}^{1,3}(641)+{}^{1,3}(551)+{}^{1,3}(542)\\
& +{}^{1,3}(632)+{}^{1,3}(542)+{}^{1,3}(533)+{}^{1,3}(542)+{}^{1,3}(443)+{}^{3,5}(731)+{}^{3,5}(641)\\
& +{}^{3,5}(632)+{}^{3,5}(641)+{}^{3,5}(551)+{}^{3,5}(542)+{}^{3,5}(632)+{}^{3,5}(542)+{}^{3,5}(533)\\
& +{}^{3,5}(533)+{}^{3,5}(443)+{}^{5,7}(542)+{}^{5,7}(443).
\end{aligned}
$$

The tableaux of $(d+s)^6$ are obtained by multiplying (411)+(330), which are of highest spin in $(d+s)^3$, by (411)+(330). If we multiply (442), which represents terms of spin 5/2 in $(d+s)^5$, by (200), we obtain the quintets and septets of $(d+s)^6$. In addition, by multiplying (431), which gives the highest spin of $(d+s)^4$, by (310), we get the triplets, quintets and septets of $(d+s)^6$. The singlets are then what remains. To check we can again compare with the known terms of $(d+s)^6$. Thus

$$
\begin{aligned}
(d+s)^6\text{:}\quad & {}^1(822)+{}^1(660)+{}^1(741)+{}^1(642)+{}^1(642)+{}^1(444)+{}^3(741)+{}^3(732)\\
& +{}^3(642)+{}^3(552)+{}^3(633)+{}^3(543)+{}^3(651)+{}^5(642)+{}^5(543)+{}^7(444)\\
(d+s)^6p\text{:}\quad & {}^2(922)+{}^2(832)+{}^2(760)+{}^2(661)+{}^2(841)+{}^2(751)+{}^2(742)+{}^2(742)\\
& +{}^2(652)+{}^2(643)+{}^2(742)+{}^2(652)+{}^2(643)+{}^2(544)+{}^{2,4}(841)+{}^{2,4}(751)\\
& +{}^{2,4}(742)+{}^{2,4}(832)+{}^{2,4}(742)+{}^{2,4}(733)+{}^{2,4}(742)+{}^{2,4}(652)+{}^{2,4}(643)\\
& +{}^{2,4}(652)+{}^{2,4}(553)+{}^{2,4}(733)+{}^{2,4}(643)+{}^{2,4}(643)+{}^{2,4}(553)+{}^{2,4}(544)\\
& +{}^{2,4}(751)+{}^{2,4}(661)+{}^{2,4}(652)+{}^{4,6}(742)+{}^{4,6}(652)+{}^{4,6}(643)+{}^{4,6}(643)\\
& +{}^{4,6}(553)+{}^{4,6}(544)+{}^{6,8}(544).
\end{aligned}
$$

Tables 2–7 give the expected eigenvalues and their multiplicities for all terms of $(d+s)^n p$, where $n \leq 6$.

TABLE 2. *Expected eigenvalues and their multiplicities for* (d + s)p

TABLEAU	(30)	(21)
Eigenvalue / Term	36	18
^1P	1	1
^1D		1
^1F	1	
^3P	1	1
^3D		1
^3F	1	

TABLE 3. *Expected eigenvalues and their multiplicities for* $(d+s)^2p$

TABLEAU	(50)	(41)	(32)	(20)	(11)
Eigenvalue / Term	80	50	32	20	8
^2S				1	
^2P	1	2	2		1
^2D		2	2	1	
^2F	1	2	2		
^2G		2			
^2H	1				
^4S				1	
^4P		1	1		
^4D		1	1	1	
^4F		1	1		
^4G		1			

TABLE 4. *Expected eigenvalues and their multiplicities for* $(d+s)^3p$

TABLEAU	(61)	(52)	(40)	(43)	(31)	(22)	(10)
Eigenvalue / Term	98	68	56	50	32	20	8
^1S			1			1	
^1P	1	2		1	2		1
^1D	1	2	1	1	2	1	
^1F	1	4		1	2		
^1G	1	2	1	1			
^1H	1	2					
^1I	1						
^3S			2			2	
^3P	1	2		2	3		1
^3D	1	2	2	2	3	2	
^3F	1	4		2	3		
^3G	1	2	2	2			
^3H	1	2					
^3I	1						
^5S			1			1	
^5P				1	1		
^5D			1	1	1	1	
^5F				1	1		
^5G			1	1			

TABLE 5. *Expected eigenvalues and their multiplicities for* $(d+s)^4p$

TABLEAU	(72)	(60)	(63)	(51)	(42)	(33)	(21)	(10)
Eigenvalue / Term	120	108	90	72	48	36	18	0
^2S		1			4			1
^2P	1		2	6		5	3	
^2D	1	1	2	6	8		3	
^2F	2		4	6	4	5		
^2G	1	1	4	6	4			
^2H	2		2	6				
^2I	1	1	2					
^2K	1							
^4S		1			4			1
^4P			1	3		3	3	
^4D		1	1	3	8		3	
^4F			2	3	4	3		
^4G		1	2	3	4			
^4H			1	3				
^4I		1	1					
^6S					1			
^6P						1	1	
^6D					2		1	
^6F					1	1		
^6G					1			

TABLE 6. *Expected eigenvalues and their multiplicities for* $(d+s)^5p$

TABLEAU	(71)	(74)	(65)	(62)	(50)	(53)	(44)	(41)	(32)	(20)	(11)
Eigenvalue / Term	128	116	98	92	80	68	56	50	32	20	8
^1S				2			1			1	
^1P	1	1	1		2	3		3	3		1
^1D	1	1	1	4		3	1	3	3	1	
^1F	1	2	1	2	2	6		3	3		
^1G	1	2	1	4		3	1	3			
^1H	1	2	1	2	2	3					
^1I	1	1	1	2							
^1K	1	1									
^3S				3			2			3	
^3P	1	1	1		2	5		5	5		2
^3D	1	1	1	6		5	2	5	5	3	
^3F	1	2	1	3	2	10		5	5		
^3G	1	2	1	6		5	2	5			
^3H	1	2	1	3	2	5					
^3I	1	1	1	3							
^3K	1	1									
^5S				1			1			2	
^5P						2		2	3		2
^5D				2		2	1	2	3	2	
^5F				1		4		2	3		
^5G				2		2	1	2			
^5H				1		2					
^5I				1							
^7P									1		1
^7D									1		
^7F									1		

TABLE 7. *Expected eigenvalues and their multiplicities for* $(d+s)^6p$

TABLEAU	(70)	(76)	(73)	(61)	(64)	(55)	(52)	(40)	(43)	(31)	(22)	(10)
Eigenvalue / Term	140	128	116	98	92	80	68	56	50	32	20	8
^2S					3			2			2	
^2P	1	1	2	2		2	6		5	5		2
^2D		1	2	2	6		6	2	5	5	2	
^2F	1	1	4	2	3	2	12		5	5		
^2G		1	4	2	6		6	2	5			
^2H	1	1	4	2	3	2	6					
^2I		1	2	2	3							
^2K	1	1	2									
^4S					2			2			3	
^4P			1	1		1	4		4	5		2
^4D			1	1	4		4	2	4	5	3	
^4F			2	1	2	1	8		4	5		
^4G			2	1	4		4	2	4			
^4H			2	1	2	1	4					
^4I			1	1	2							
^4K			1									
^6S											1	
^6P							1		1	2		2
^6D							1		1	2	1	
^6F							2		1	2		
^6G							1		1			
^6H							1					
^8P												1

3. The Parameters of the Casimir Check

Following Racah [18], we define the tensor operator $u^{(k)}$ by

$$(nl||u^{(k)}||n'l') = \delta_{nn'}\,\delta_{ll'}.$$

Then let

$$U_q^{(k)} = \sum_{i=1}^{n} u_q^{(k)}[i],$$

where i refers to the ith of n electrons.

The group SU_{2l+1} is formed by the $4l(l+1)$ tensor operators $U_q^{(k)}$ where $-k \leq q \leq k$ and $1 \leq k \leq 2l$. Thus the group SU_3 is formed by the eight operators $U_{-1}^{(1)}$, $U_0^{(1)}$, $U_1^{(1)}$, $U_{-2}^{(2)}$, $U_{-1}^{(2)}$, $U_0^{(2)}$, $U_1^{(2)}$, and $U_2^{(2)}$. From equation (5–48) of Judd [19], we have for the Casimir operator of SU_3

$$\begin{aligned} G(SU_3) &= \tfrac{1}{6}\{3[U^{(1)}]^2 + 5[U^{(2)}]^2\} \\ &= \tfrac{1}{6}\left\{3[U^{(1)}]^2 + 5\sum_{i=1}^{n}[u^{(2)}[i]]^2 + 10\sum_{i<j} u^{(2)}[i]\cdot u^{(2)}[j]\right\}. \end{aligned} \tag{3}$$

From the above expression we can immediately obtain which parameters enter the Casimir check. From equation (103) of Racah [18], the first contribution is proportional to $L(L+1)$, and thus the parameter λ must be included. The second term is a constant and is responsible for an additive term for each electron of a given l. The last contribution is a sum of products of tensors of second order and therefore only Slater parameters with k equal to 2 enter the Casimir check. These are $F_2(dd)$ or B, $F_2(dp)$, G'_{ds}, H, and J.

If E_s, E_p, and E_d are the additive constants for the electrons s, p, and d respectively, then from table 1,

$$^2\mathrm{S} = E_s = 20 \tag{4}$$

$$^2\mathrm{P} = E_p + 2\lambda = 8 \tag{5}$$

$$^2\mathrm{D} = E_d + 6\lambda = 20. \tag{6}$$

As the parameters A and C do not enter the Casimir check we have from (78) RII [1], the tableaux of $(d+s)^2$ and table 1,

$$d^2\ ^3\mathrm{P} = 2E_d + 7B + 2\lambda = 32 \tag{7}$$

$$d^2\ ^3\mathrm{F} = 2E_d - 8B + 12\lambda = 32 \tag{8}$$

$$d^2\ ^1\mathrm{G} = 2E_d + 4B + 20\lambda = 56. \tag{9}$$

Solving (7), (8), and (9) yields

$$E_d = 11, \qquad B = 1, \qquad \text{and } \lambda = \tfrac{3}{2}. \tag{10}$$

Then, from (5)

$$E_p = 5. \tag{11}$$

From p. 197, [3] and the tableau for $ds\ ^3\mathrm{D}$ we have

$$ds\ ^3\mathrm{D} = E_d + E_s - G'_{ds} + 6\lambda = 32. \tag{12}$$

Inserting the values for E_d, E_s, and λ from (4) and (10) yields

$$G'_{ds} = 8. \tag{13}$$

From (78) RII [1] and p. 197, [3]

$$ds\ ^1\mathrm{D} = E_d + E_s + G'_{ds} + 6\lambda \tag{14}$$

$$d^2\ ^1\mathrm{D} = 2E_d - 3B + 6\lambda. \tag{15}$$

Then, from (4), (10), and (13), we have

$$ds\ ^1\mathrm{D} = 48 \tag{16}$$

$$d^2\ ^1\mathrm{D} = 28. \tag{17}$$

Now, the interaction between $d^2\ ^1\mathrm{D}$ and $ds\ ^1\mathrm{D}$ is given by $-2\sqrt{35}\ H$, [20].
Then from (16) and (17), the eigenvalues of the matrix for $^1\mathrm{D}$ are

$$38 \pm \sqrt{100 + 140H^2}.$$

Since, from the tableaux of $(d+s)^2$, and table 1, these eigenvalues should equal 20 and 56, H is given by

$$H = \sqrt{40}/5. \tag{18}$$

The parameter G is the same as the parameter G'_{ds} [2], and thus should also have a value equal to 8. This result can be checked in the following manner.
Using (78) RII and the tableaux of $(d+s)^2$ we have

$$d^2\ ^1\mathrm{S} = 2E_d + 14B = 36 \tag{19}$$

$$s^2\ ^1\mathrm{S} = 2E_s = 40. \tag{20}$$

From (75) RIII the interaction between d^2 and s^2 is given by $\sqrt{5}\ G$. Thus, from (19) and (20), the eigenvalues of the matrix for $^1\mathrm{S}$ are $38 \pm \sqrt{4 + 5G^2}$. Since the predicted eigenvalues are 20 and 56, we obtain

$$G = 8. \tag{21}$$

From p. 200 TAS, the tableau for $dp\ ^1\mathrm{F}$ and table 1, we have

$$dp\ ^1\mathrm{F} = E_d + E_p + 2F_2 + 12\lambda = 36.$$

By using (10) and (11)

$$F_2 = 1. \tag{22}$$

Again from p. 200 TAS

$$dp\ ^1\mathrm{P} = E_d + E_p + 7F_2 + 2\lambda. \tag{23}$$

From (10), (11), and (22) we obtain

$$dp\ ^1\mathrm{P} = 26. \tag{24}$$

Similarly,

$$sp\ ^1\mathrm{P} = E_s + E_p + 2\lambda = 28. \tag{25}$$

By (7) Ref. [11], the interaction between $dp\ ^1P$ and $sp\ ^1P$ is given by $-(J+K)\sqrt{2}$.

As K is a Slater parameter with k equal to 1 it does not enter the Casimir check. Then from (24) and (25), the eigenvalues of ^1P are given by

$$27 \pm \sqrt{1+2J^2}.$$

Since the predicted eigenvalues are 18 and 36, we obtain

$$J = 2\sqrt{10}. \tag{26}$$

If we now consider $(d+s)^n p$ we have

$$\begin{aligned} A(d^n p) &= nE_d + E_p \\ &= 11n + 5 \end{aligned} \tag{27}$$

$$\begin{aligned} S' &= A'(d^{n-1}sp) - A(d^n p) \\ &= (n-1)E_d + E_s + E_p - nE_d - E_p \\ &= E_s - E_d = 9. \end{aligned} \tag{28}$$

In the configuration $d^{n-2}s^2p$ we must also take into account the exchange interaction between the electrons d and s which is given by $-(n-2)G'_{ds}$, [11]. This is a constant for each term of $d^{n-2}s^2p$ and thus the matrix multiplying G'_{ds} is not put on tape, but must be added to the height of the configuration.

Thus,

$$\begin{aligned} S'' &= A''(d^{n-2}s^2p) - A(d^n p) \\ &= (n-2)E_d + 2E_s + E_p - (n-2)G_{ds} - nE_d - E_p \\ &= -2E_d + 2E_s - (n-2)8 \\ &= 34 - 8n. \end{aligned} \tag{29}$$

Thus, we have the following parameters for the Casimir check of $(d+s)^n$:

$$\begin{aligned} A &= 11n + 5 \\ S' &= 9 \\ S'' &= 34 - 8n \\ B &= B' = B'' = 1 \\ G'_{ds} &= G = 8 \\ F_2 &= F'_2 = F''_2 = 1 \\ H &= H' = \sqrt{40}/5 \\ J &= J' = 2\sqrt{10} \\ \lambda &= \lambda' = \lambda'' = \tfrac{3}{2}. \end{aligned} \tag{30}$$

The other parameters equal zero.

If we take into consideration only the parameters which enter the Casimir check, we have from eqs (1) and (2) p. 296 TAS and eqs (11) and (12) pp. 182, 183 TAS, that the difference between the configurations d^6p and d^4p is given by

$$-(25/2)C_{222}F^2(dd) - [(-4\times 5)/2]C_{222}F^2(dd).$$

By eq (9) p. 182, TAS, the above expression reduces to $-(2/7)F^2(d,d)$ which equals $-14B$ here. Since the matrices of B for d^6p which we used are the same as those of d^4p, the above contribution must be incorporated into the height of the configuration d^6p.

Then, for $(d+s)^6p$

$$A(d^6p) = 6E_d + E_p - 14B = 66 + 5 - 14 = 57$$
$$A'(d^5sp) = 5E_d + E_s + E_p = 80$$
$$S' = 80 - 57 = 23$$
$$A''(d^4s^2p) = 4E_d + 2E_s + E_p - 4G'_{ds}$$
$$= 57$$
$$S'' = 0.$$

4. The Casimir Check for $(d+s)^np$, $n > 6$

The configuration $(d+s)^{12}$ consists of the single term $d^{10}s^2\ {}^1S$. In this case $p+q+r$ equals 24, and thus the Young's tableau for $(d+s)^{12}$ must be (8, 8, 8). Now, $(d+s)^n$ and $(d+s)^{12-n}$ together form $(d+s)^{12}$. Thus, if the Young's tableaux of $(d+s)^{12-n}$ are (p, q, r), then the tableaux for $(d+s)^n$ are $(8-r, 8-q, 8-p)$ since in (p, q, r), r has the smallest number of blocks so that $(8-r)$ has the largest number. The configuration $(d+s)^6$ is self-complementary. For $(d+s)^np$, the p electron is then added to any row as long as $p \geq q \geq r$.

In Ref. [11] it was shown that for $n > 6$, it is only necessary to calculate the matrices of the parameters G'_1, G'_3, K, and K'. However, none of these parameters enter the Casimir check and thus we only need this check for $n \leq 6$. It is, nevertheless, instructive to obtain the Young's tableaux for at least one case when $n > 6$. Thus, we consider the configuration $(d+s)^{10}p$. Since the tableaux of $(d+s)^2$ are

$$^1(40) + {}^1(22) + {}^3(31),$$

the tableaux of $(d+s)^{10}$ are

$$^1(884) + {}^1(866) + {}^3(875).$$

We note that the expected eigenvalues are the same as those of $(d+s)^2$. This is generally true because the only difference between $(d+s)^n$ and $(d+s)^{12-n}$ is a change in sign of the matrices of H, for n even. However, changing the sign of all the matrix elements of the interactions $d^n - d^{n-1}s$, and $d^{n-1}s - d^{n-2}s^2$ is equivalent to changing the sign of the rows and columns of $d^{n-1}s$. This transformation evidently does not change the eigenvalues. That the eigenvalues of the Casimir check for the configurations $(d+s)^n$ and $(d+s)^{12-n}$ are the same can also be seen from (2), as generally

$$g(p, q, r) = g(a-r, a-q, a-p).$$

Thus, specifically, for $(d+s)^n$ and $(d+s)^{12-n}$

$$g(p, q, r) = g(8-r, 8-q, 8-p).$$

However, the tableaux of $(d+s)^{10}p$ are

$$^2(54) + {}^2(33) + {}^2(30) + {}^2(21) + {}^{2,4}(42) + {}^{2,4}(33) + {}^{2,4}(21).$$

We note that the expected eigenvalues differ from those of $(d+s)^2p$. This is because when going from $(d+s)^np$ to $(d+s)^{12-n}p$ the matrices of the parameters F_2, F'_2, and F''_2 change sign. This change in sign affects the diagonal elements also and is sufficient to cause the eigenvalues to change.

In addition, the matrices of either J and J' or H and H' change sign as we go from $(d+s)^n p$ to $(d+s)^{12-n}p$. Thus, in the Casimir check not only are the matrix elements of the interaction between configurations in $(d+s)^n p$ of different sign than those of $(d+s)^{12-n}p$, but they also differ in magnitude.

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Convex Homotopy

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Given any two continuous, convex functions f and g on a compact, convex set with certain properties ("regular" convexity), it is shown that an infinite number of homotopies of f and g exist which are also convex. One such homotopy in particular (the "basic" homotopy) is shown to have nice monotonicity properties and can be used as a basis for constructing other homotopies. A method of constructing the basic homotopy is given for the case where the domain of f and g is a line segment. (Theorems are for normed linear spaces only.)

Key words: Convex functions; convex sets; homotopy.

1. Introduction

In a normed linear space, a set C is called *convex* if $\lambda x+\bar{\lambda}y \in C$ for every $x, y \in C$ and every λ with $0 \leq \lambda \leq 1$, where $\bar{\lambda}=1-\lambda$. (We shall use the notation of a bar over a quantity to denote $1-$(that quantity) throughout the rest of this paper.) A mapping f of C into the reals is called *convex* if

$$f(\lambda x+\bar{\lambda}y) \leq \lambda f(x)+\bar{\lambda}f(y)$$

for all $x, y \in C$ and $0 \leq \lambda \leq 1$. Given any two continuous convex maps f and g on C, we define a map

$$h: C \times [a, b] \to R,$$

where $-\infty < a < b < \infty$ and R is the real numbers, to be a convex homotopy of (f, g) if h is a continuous convex map and $h(x, a)=f(x)$, $h(x, b)=g(x)$, for all $x \in C$. (Usually $a=0$ and $b=1$ in the definition of homotopy, but this definition will simplify notation and is equivalent to the usual definition.)

The question arises whether any two continuous convex maps f and g can be connected by a convex homotopy and, if so, how many such homotopies exist and what are their properties. The following gives an affirmative answer to the basic question for certain types of domain sets and shows that there are always an infinite number of such homotopies. Certain characteristics of a "basic" convex homotopy are also derived.

It will be noted in the following that proofs of continuity are, for the most part, independent of convexity, and it would be possible to construct a "not-necessarily-continuous" convex homotopy of two maps, using the following procedures, with much less stringent conditions on the maps and their domain. This observation might lead to inquiry about the existence of convex sets given a specification of part of their boundaries. This idea will not be pursued here.

The reader is also referred to an article by Victor Klee [1] which contains results similar to those of theorems 1, 2, and 4, without the concept of continuity.

AMS Subject Classification: Primary 5225, Secondary 5540.

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2. Existence; Basic and Other Homotopies

We define a *regularly convex* set C to be a convex set with the following property. For each $x\epsilon C$, $\epsilon > 0$, and $0 \leq \lambda \leq 1$, there exists $\delta(x, \epsilon, \lambda) > 0$ such that if y and z are any points of C for which

$$x = \lambda y + \bar{\lambda} z,$$

then for any point $x'\epsilon C$ with $\|x - x'\| < \delta$ there exist points $y', z'\epsilon C$ such that

$$x' = \lambda y' + \bar{\lambda} z'$$

and $\|y - y'\| < \epsilon$, $\|z - z'\| < \epsilon$. Not all convex sets are regularly convex, as will be shown by an example later, although all of the usual ones (e.g., line segment, disk in the plane) seem to be.

Given any pair of continuous convex maps f and g on a compact, regularly convex subset C of a normed linear space, let

$$H: C \times [0, 1] \to R$$

be defined by

$$H(x, r) = \inf \{rg(y) + \bar{r}f(z): y, z\epsilon C, x = ry + \bar{r}z\}.$$

(H, of course, is dependent on f and g, but this dependence will not be indicated unless necessary for clarity.)

THEOREM 1: *For* f, g, *and* C *as above,* H *is a convex homotopy of* (f, g) *on* $C \times [0, 1]$. *Furthermore, if* h *is any other such homotopy, then* $h(x, r) \leq H(x, r)$ *for all* $x\epsilon C$, $r\epsilon[0, 1]$.

PROOF: First, it is clear that $H(x, 0) = f(x)$ and $H(x, 1) = g(x)$, by the definition of H. It remains to show that H is convex and continuous.

Let (x, r) and (y, s) be any two points of $C \times [0, 1]$, with r and s not both 0 or 1. If x_1, x_2, y_1, and y_2 are any points of C such that $x = rx_1 + \bar{r}x_2$ and $y = sy_1 + \bar{s}y_2$, then for any λ with $0 < \lambda < 1$ we have

$$\begin{aligned}
\lambda(x, r) + \bar{\lambda}(y, s) &= (\lambda x + \bar{\lambda} y,\ \lambda r + \bar{\lambda} s) = (\lambda r x_1 + \lambda \bar{r} x_2 + \bar{\lambda} s y_1 + \bar{\lambda} \bar{s} y_2,\ \lambda r + \bar{\lambda} s) \\
&= \left([\lambda r + \bar{\lambda} s] \frac{\lambda r x_1 + \bar{\lambda} s y_1}{\lambda r + \bar{\lambda} s} + [\lambda \bar{r} + \bar{\lambda} \bar{s}] \frac{\lambda \bar{r} x_2 + \bar{\lambda} \bar{s} y_2}{\lambda \bar{r} + \bar{\lambda} \bar{s}},\ \lambda r + \bar{\lambda} s \right) \\
&= (\mu [a_1 x_1 + \bar{a}_1 y_1] + \bar{\mu} [a_2 x_2 + \bar{a}_2 y_2],\ \mu),
\end{aligned}$$

where

$$\mu = \lambda r + \bar{\lambda} s,$$

$$a_1 = \frac{\lambda r}{\mu},$$

$$a_2 = \frac{\lambda \bar{r}}{\bar{\mu}}.$$

Thus,

$$H(\lambda(x, r) + \bar{\lambda}(y, s)) = H((\mu [a_1 x_1 + \bar{a}_1 y_1] + \bar{\mu} [a_2 x_2 + \bar{a}_2 y_2],\ \mu)) \leq \mu g(a_1 x_1 + \bar{a}_1 y_1) + \bar{\mu} f(a_2 x_2 + \bar{a}_2 y_2)$$

(by the definition of H)

$$\leq \mu a_1 g(x_1) + \mu \bar{a}_1 g(y_1) + \bar{\mu} a_2 f(x_2) + \bar{\mu} \bar{a}_2 f(y_2)$$

(by the convexity of f and g)

$$= \lambda r g(x_1) + \bar{\lambda} s g(y_1) + \lambda \bar{r} f(x_2) + \bar{\lambda} \bar{s} f(y_2)$$

$$= \lambda [r g(x_1) + \bar{r} f(x_2)] + \bar{\lambda} [s g(y_1) + \bar{s} f(y_2)].$$

Since x_1, x_2, y_1 and y_2 were chosen arbitrarily, satisfying only the conditions

$$x = r x_1 + \bar{r} x_2 \text{ and } y = s y_1 + \bar{s} y_2,$$

it follows that

$$H(\lambda(x, r) + \bar{\lambda}(y, s)) \leq \inf \{\lambda(r g(x_1) + \bar{r} f(x_2)) : x_1, x_2 \epsilon C \text{ and } x = r x_1 + \bar{r} x_2\}$$
$$+ \inf \{\bar{\lambda}(s g(y_1) + \bar{s} f(y_2)) : y_1, y_2 \epsilon C \text{ and } y = s y_1 + \bar{s} y_2\} = \lambda H(x,r) + \bar{\lambda} H(y,s),$$

proving convexity of H.

A proof of continuity of H is as follows. First, we define a norm on $C \times [0, 1]$ as the sum of the norms on C and $[0, 1]$.

That is,

$$\|(x, r), (y, s)\| = \|x - y\| + |r - s|.$$

Next, note if C is regularly convex, then $C \times [0, 1]$ is also regularly convex. For, given $(x, r) \epsilon C \times [0, 1]$, $0 \leq \lambda \leq 1$, and $\epsilon > 0$, if

$$(x, r) = \lambda(y, s) + \bar{\lambda}(z, t),$$

then there exists $\delta > 0$ such that, if $x' \epsilon C$ and $\|x - x'\| < \delta$, then there exist y' and z' such that

$$x' = \lambda y' + \bar{\lambda} z',$$

where $\|y - y'\| < \epsilon/2$, $\|z - z'\| < \epsilon/2$. Thus if

$$\|(x, r) - (x', r')\| < \delta$$

and, say, $s < r < t$, while $r' > r$, we merely take

$$t' = t$$

and

$$s' = s + \frac{r' - r}{\lambda}$$

(where δ is chosen small enough so that $r', s' \epsilon [s, t]$ and $|s - s'| < \epsilon/2$). Of course, if $\lambda = 0$ we take $s' = s$, $t' = r'$. A similar construction is followed if $r' < r$.

It is clear, then, that the points (y', s') and (z', t') satisfy the conditions

$$(x', r') = \lambda(y', s') + \bar{\lambda}(z', t'),$$

$\|(y, s) - (y', s')\| < \epsilon$, $\|(z, t) - (z', t')\| < \epsilon$. Thus $C \times [0, 1]$ is also regularly convex.

The proof of continuity of H will be given first for points $(x, 0)$ and $(x, 1)$, and then for other points.

Given any point (say) $(x, 0)$, if (y, s) is any point for which

$$\|(x, 0) - (y, s)\| < \delta,$$

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for some $\delta > 0$, then $s < \delta$. Let u and v be two points of C for which

$$y = su + \bar{s}v,$$

and

$$H(y, s) = sg(u) + \bar{s}f(v).$$

(Such points exist by the compactness of C.) Then

$$s(y-u) = \bar{s}(v-y),$$

or

$$\|v-y\| = \frac{s}{\bar{s}}\|y-u\| \leq 2\delta D,$$

if $\delta < 1/2$, where D is an upper bound on the distance between pairs of points of C. Thus,

$$|H(y, s) - H(x, 0)| = |sg(u) + \bar{s}f(v) - f(x)|$$

$$\leq s|g(u)| + \bar{s}|f(v) - f(y)| + \bar{s}|f(y) - f(x)| + s|f(x)| \to 0 \text{ as } \delta \to 0.$$

Thus H is continuous for each $(x, 0)$ (and also for each $(x, 1)$).

Now let (x, r) be any point of $C \times [0, 1]$. We will show that, if $\{(x_n, r_n)\}$ is a sequence converging to (x, r), then

$$H(x, r) \leq \liminf H(x_n, r_n),$$

and

$$\limsup H(x_n, r_n) \leq H(x, r).$$

First, let $\{(x_{n_i}, r_{n_i})\}$ be any subsequence of $\{(x_n, r_n)\}$ such that

$$H(x_{n_i}, r_{n_i}) \to \liminf H(x_n, r_n).$$

By the compactness of C, for each (x_{n_i}, r_{n_i}) there exist points y_{n_i} and z_{n_i} in C such that

$$x_{n_i} = r_{n_i} y_{n_i} + \bar{r}_{n_i} z_{n_i},$$

$$H(x_{n_i}, r_{n_i}) = r_{n_i} g(y_{n_i}) + \bar{r} f(z_{n_i}).$$

By the compactness of $C \times [0, 1]$, there exists a subsequence of $\{(x_{n_i}, r_{n_i})\}$, which we assume for convenience to be $\{(x_{n_i}, r_{n_i})\}$ itself, and points $y, z \in C$, such that

$$y_{n_i} \to y,$$

$$z_{n_i} \to z,$$

while

$$x = \lim x_{n_i} = \lim (r_{n_i} y_{n_i} + \bar{r}_{n_i} z_{n_i}) = ry + \bar{r}z.$$

But then

$$H(x, r) \leq rg(y) + \bar{r}f(z) = \lim (r_{n_i} g(y_{n_i}) + \bar{r}_{n_i} f(z_{n_i}))$$

$$= \liminf H(x_{n_i}, r_{n_i}),$$

proving the first part.

Now let u and v be two points of C such that

$$x = ru + \bar{r}v,$$

$$H(x, r) = rg(u) + \bar{r}f(v).$$

(Such points exist by the compactness of C.) By the regular convexity of $C \times [0, 1]$, given $\epsilon > 0$ there exists $\delta > 0$ such that for any point (w, s) with

$$\|(w, s) - (x, r)\| < \delta,$$

there exist points (w_1, s_1) and (w_2, s_2), such that

$$(w, s) = r(w_1, s_1) + \bar{r}(w_2, s_2),$$

and

$$\|(w_1, s_1) - (u, 1)\| < \epsilon,$$

$$\|(w_2, s_2) - (v, 0)\| < \epsilon.$$

But the convexity of H implies

$$H(w, s) \leq rH(w_1, s_1) + \bar{r}H(w_2, s_2).$$

By the continuity of H at $(u, 1)$ and $(v, 0)$,

$$H(w, s) \leq rH(u, 1) + \bar{r}H(v, 0) + \eta = H(x, r) + \eta,$$

where $\eta > 0$, $\eta \to 0$ as $\epsilon \to 0$. Thus, for a given $\eta > 0$, there exists $\delta > 0$ such that

$$H(w, s) \leq H(x, r) + \eta$$

whenever $\|(w, s) - (x, r)\| < \delta$.

Applying this inequality to the sequence $\{(x_n, r_n)\}$, we have

$$H(x_n, r_n) \leq H(x, r) + \eta,$$

when $\|(x, r) - (x_n, r_n)\| < \delta$, and hence

$$\limsup H(x_n, r_n) \leq H(x, r).$$

Since

$$\liminf H(x_n, r_n) \leq \limsup H(x_n, r_n),$$

it follows that

$$H(x, r) = \lim H(x_n, r_n),$$

and hence that H is continuous on $C \times [0, 1]$.

Finally, if h is any other convex homotopy of (f, g), then

$$h(x, r) \leq rh(y, 1) + \bar{r}h(z, 0) = rg(y) + \bar{r}f(z)$$

for any $y, z \in C$ such that $x = ry + \bar{r}z$. Thus

$$h(x, r) \leq H(x, r).$$

This completes the proof of theorem 1.

We shall call the map H the *basic* convex homotopy of (f, g) on $C \times [0, 1]$. A basic convex homotopy H' on $C \times [a, b]$ is defined by

$$H'(x, r) = H\left(x, \frac{r-a}{b-a}\right).$$

At this point it is appropriate to give examples of convex sets which are not compact or not regularly convex, and show that the H defined for a given f and g need not be continuous.

First, let C be the set of points in the plane defined by

$$C = \{(0, 0)\} \cup \{(x, y) : 0 < x < 1, -1 < y < 1\},$$

and let $f(x, y) = y$ and $g(x, y) = -y$. Then for every $(x, 0)$ except $(0, 0)$, we have

$$H((x, 0), \tfrac{1}{2}) = \tfrac{1}{2}f(x, -1) + \tfrac{1}{2}g(x, 1) = -1$$

while

$$H((0, 0), \tfrac{1}{2}) = \tfrac{1}{2}f(0, 0) + \tfrac{1}{2}g(0, 0)$$

$$= 0.$$

For the next example, let C be the convex hull of the set of points in three-space

$$C' = \{(0, 0, -1)\} \cup \{(0, 0, 1)\} \cup \{(x, y, 0) : y = x^2, y \leq 1\}.$$

Then C is clearly the union of two convex cones, from $(0, 0, -1)$ and $(0, 0, 1)$ respectively, to the set

$$\{(x, y, 0) : x^2 \leq y \leq 1\}.$$

Let $f(x, y, z) = z$, while $g(x, y, z) = -z$. Again, for $x \neq 0$ we have

$$H((x, x^2, 0), \tfrac{1}{2}) = \tfrac{1}{2}f(x, x^2, 0) + \tfrac{1}{2}g(x, x^2, 0)$$

$$= 0,$$

while

$$H((0, 0, 0), \tfrac{1}{2}) = \tfrac{1}{2}f(0, 0, -1) + \tfrac{1}{2}g(0, 0, 1)$$

$$= -1.$$

Next we show that the basic convex homotopy is by no means the only convex homotopy joining two convex maps. From this point onward in the discussion we shall use the term "convex map" to refer only to a continuous, convex map on a compact, regularly convex domain set.

THEOREM 2: *Let* f, g, *and* h *be convex maps on* C *satisfying*

$$h(x) \leq H(x, r)$$

for all $x \in C$, *where* H *is the basic convex homotopy of* (f, g) *and* r *is some constant such that* $0 < r < 1$. *Let* H_1 *and* H_2 *be the basic convex homotopies of* (f, h) *and* (h, g) *on* $C \times [0, r]$ *and* $C \times [r, 1]$, *respectively. If* G *is the map defined by*

$$G(x, s) = H_1(x, s), \qquad 0 \leq s \leq r$$

and

$$G(x, s) = H_2(x, s), \qquad r \leq s \leq 1,$$

then G *is convex and hence is a convex homotopy of* (f, g).

PROOF: It is clear that if (x, s) and (y, t) are two points of $C \times [0, 1]$ such that $s, t < r$ or $s, t > r$, then

$$G(\lambda(x, s) + \bar{\lambda}(y, t)) \leq \lambda G(x, s) + \bar{\lambda} G(y, t)$$

by the convexity of H_1 or H_2. It remains to show that the above inequality holds when s and t are on different sides of r.

Suppose $s < r$ and $t > r$. Let

$$m = \frac{t-r}{t-s},$$

$$p = \frac{s}{r},$$

$$q = \frac{t-r}{\bar{r}}.$$

If x_1, x_2, y_1, and y_2 are points of C such that

$$x = px_1 + \bar{p}x_2$$

and

$$y = qy_1 + \bar{q}y_2,$$

then we have

$$\begin{aligned}
&m[ph(x_1) + \bar{p}f(x_2)] + \bar{m}[qg(y_1) + \bar{q}h(y_2)] \\
&= [m\bar{p}f(x_2) + \bar{m}qg(y_1)] + mph(x_1) + \bar{m}\bar{q}h(y_2) \\
&= (m\bar{p} + \bar{m}q)[\bar{r}f(x_2) + rg(y_1)] + mph(x_1) + \bar{m}\bar{q}h(y_2) \\
&\geq (m\bar{p} + \bar{m}q)h(\bar{r}x_2 + ry_1) + mph(x_1) + \bar{m}\bar{q}h(y_2) \\
&\qquad \text{(by the fact that } h \leq H(\cdot, r)) \\
&\geq h([m\bar{p} + \bar{m}q][\bar{r}x_2 + ry_1] + mpx_1 + \bar{m}\bar{q}y_2) \\
&\qquad \text{(by the convexity of } h) \\
&= h(m\bar{p}x_2 + \bar{m}qy_1 + mpx_1 + \bar{m}\bar{q}y_2) \\
&= h(mx + \bar{m}y) \\
&= G(mx + \bar{m}y, r).
\end{aligned}$$

Therefore, since x_1, x_2, y_1, and y_2 were arbitrary, satisfying only $x = px_1 + \bar{p}x_2$ and $y = qy_1 + \bar{q}y_2$,

$$\begin{aligned}
mG(x, s) + \bar{m}G(y, t) &= m \inf \{ph(x_1) + \bar{p}f(x_2) : x_1, x_2 \in C, x = px_1 + \bar{p}x_2\} \\
&\quad + \bar{m} \inf \{qg(y_1) + \bar{q}h(y_2) : y_1, y_2 \in C, y = qy_1 + \bar{q}y_2\} \\
&\qquad \text{(see definition after theorem 1)} \\
&\geq G(mx + \bar{m}y, r),
\end{aligned}$$

noting $ms + \bar{m}t = r$.

This establishes the convexity condition on (x, s) and (y, t) for the critical point $\lambda = m$, where the second coordinate becomes r. To prove it for any other λ, let us take (say) $0 < \lambda < m$. Then

$$\lambda G(x, s) + \bar{\lambda} G(y, t) = \frac{\lambda}{m} [mG(x, s) + \bar{m} G(y, t)] + \left(1 - \frac{\lambda}{m}\right) G(y, t)$$

$$\geqslant \frac{\lambda}{m} G(m(x, s) + \bar{m}(y, t)) + \left(1 - \frac{\lambda}{m}\right) G(y, t)$$

$$\geqslant G\left(\frac{\lambda}{m} [m(x, s) + \bar{m}(y, t)] + \left(1 - \frac{\lambda}{m}\right) (y, t)\right)$$

(by the convexity of H_2)

$$= G(\lambda(x, s) + \bar{\lambda}(y, t)).$$

A similar argument holds when $\lambda > m$.

This completes the proof of the convexity of G.

COROLLARY 3: *If* $h = H(\cdot, r)$ *in theorem 2, then* $G = H$.

PROOF. Because G is a convex homotopy of (f, g), we have $G \leqslant H$, by theorem 1. But because $G = H_1$ on $C \times [0, r]$ and $G = H_2$ on $C \times [r, 1]$, the basic convex homotopies on these sets, whereas H is another homotopy of $(f, H(\cdot, r))$ on $C \times [0, r]$ and of $(H(\cdot, r), g)$ on $C \times [r, 1]$, we must have $H \leqslant G$.

THEOREM 4: *Let* $f_0, f_1, \ldots, f_n$ *be convex maps defined on the set* C, *and* $0 = r_0 < r_1 < \ldots < r_n = 1$ *be a set of numbers in the unit interval. Denote by* H_{ij} *the basic convex homotopy of* (f_i, f_j) *on* $C \times [r_i, r_j]$.

If

$$f_i(x) \leqslant H_{i-1, i+1}(x, r_i)$$

for all $x \in C$ *and* $i = 1, 2, \ldots, n-1$, *then there exists a convex homotopy* G *on* $C \times [0, 1]$ *such that*

$$f_i(x) = G(x, r_i)$$

for all $x \in C$.

PROOF: Let $G(x, r) = H_{i, i+1}(x, r)$ for $r_i \leqslant r \leqslant r_{i+1}$. The proof is by induction on n.

First, for $n = 2$, the theorem is true by theorem 2. Now assume that the theorem has been proved for $n = 2, 3, \ldots, N-1$. Let (x, r) and (y, s) be any points in $C \times [0, 1]$. In order to show convexity for $n = N$, we must prove that

$$G(\lambda(x, r) + \bar{\lambda}(y, s)) \leqslant \lambda G((x, r)) + \bar{\lambda} G((y, s)),$$

for $0 < \lambda < 1$. By the induction hypothesis, it is only necessary to consider the case where $r_0 \leqslant r \leqslant r_1$ and $r_{N-1} \leqslant s \leqslant r_N$. To simplify notation, let

$$g(t) = G(ax + \bar{a}y, t),$$

where $r < t < s$ and a is such that $t = ar + \bar{a}s$. Let

$$p = \frac{r_2 - r_1}{r_2 - r}$$

and

$$q = \frac{s - r_2}{s - r_1}.$$

Then

$$g(r_1) \leq pg(r) + \bar{p}g(r_2)$$

and

$$g(r_2) \leq qg(r_1) + \bar{q}g(s),$$

by the induction hypothesis. Multiplying the first inequality by $1/(1-q+pq)$ and the second by $\bar{p}/(1-q+pq)$ and adding, we have

$$g(r_1) \leq \frac{pg(r)}{1-q+pq} + \frac{\bar{q}\bar{p}g(s)}{1-q+pq},$$

or

$$g(r_1) = g(\nu r + \bar{\nu}s) \leq \nu g(r) + \bar{\nu}g(s),$$

where

$$\nu = \frac{p}{1-q+pq},$$

proving the convexity inequality for $\lambda = \nu$. To prove the inequality for other values of λ, we use the same technique which was applied in theorem 2. Thus if $\lambda < \nu$, for instance, we write

$$\begin{aligned}
\lambda g(r) + \bar{\lambda}g(s) &= \frac{\lambda}{\nu}(\nu g(r) + \bar{\nu}g(s)) + \left(1 - \frac{\lambda}{\nu}\right) g(s) \\
&\geq \frac{\lambda}{\nu} g(r_1) + \left(1 - \frac{\lambda}{\nu}\right) g(s) \\
&\geq g\left(\frac{\lambda}{\nu} r_1 + \left(1 - \frac{\lambda}{\nu}\right)s\right) \\
&= g(\lambda r + \bar{\lambda}s),
\end{aligned}$$

by using the convexity of g on $[r_1, s]$. This completes the proof.

Theorem 4 shows a method of constructing a homotopy between two given maps which has certain desired intermediate values. We shall call a convex map G on $C \times [0, 1]$, as in the above, a *piecewise basic* convex homotopy if G is the basic homotopy of some pair (f_i, f_{i+1}) on each set $C \times [r_i, r_{i+1}]$, where $0 = r_0 < r_1 < \cdots < r_n = 1$. The next theorem shows that any convex homotopy of maps on a convex set can be approximated by a piecewise basic convex homotopy.

THEOREM 5: *Let* f *and* g *be any convex maps on the set* C, *and let* G *be a convex homotopy of* (f, g) *on* $C \times [0, 1]$. *Then there exist piecewise basic convex homotopies* $G_1, G_2, \ldots$, *such that* $G_i \to G$ *uniformly.*

PROOF: Let $M_i = \{0, r_1, r_2, \ldots, r_m = 1\}$ be finite subsets of the unit interval, where mesh $(M_i) \to 0$. For any i, if $r_j < r_{j+1} < r_{j+2}$ are any three neighboring points of M_i, we note that

$$G(x, r_{j+1}) \leq H_{j,j+2}(x, r_{j+1}),$$

where $H_{j,j+2}$ is the basic convex homotopy of $(G(\cdot, r_j), G(\cdot, r_{j+2}))$ on $C \times [r_j, r_{j+2}]$. Thus if G_i is defined to be the piecewise convex homotopy of theorem 4 with points $0 = r_0 < r_1 < \cdots < r_{m_i} = 1$ and

$$f_j = G(\cdot, r_j),$$

then G_i is indeed convex, by theorem 4.

Now for any $\epsilon > 0$, there exists $\delta > 0$ such that

$$|G(x, r) - G(x, r')| < \epsilon$$

whenever $|r-r'|<\delta$, for all $x\epsilon C$, by the compactness of $C\times[0,1]$. By taking mesh $(M_i)<\delta$, we have, for any r such that $r_j\leq r\leq r_{j+1}$,

$$G(x,r)\leq G_i(x,r)\leq \lambda G(x,r_{j+1})+\bar{\lambda}G(x,r_j),$$

where $r=\lambda r_{j+1}+\bar{\lambda}r_j$. Thus, since

$$|G(x,r)-[\lambda G(x,r_{j+1})+\bar{\lambda}G(x,r_j)]|\leq \lambda|G(x,r)-G(x,r_{j+1})|+\bar{\lambda}|G(x,r)-G(x,r_j)|$$

$$<\lambda\epsilon+\bar{\lambda}\epsilon=\epsilon,$$

we have

$$|G(x,r)-G_i(x,r)|<\epsilon,$$

proving the theorem.

Finally, we note that forming a basic convex homotopy is a continuous process in f and g.

Given two convex maps f and g, let $\mathscr{H}$ be the operator defined as: $\mathscr{H}(f,g)$ is the basic homotopy H_{fg} of (f,g) on $C\times[0,1]$, where C is the domain set of f and g. Then $\mathscr{H}$ maps pairs of functions on C into functions on $C\times[0,1]$. We shall use the sup norm for all functions in the following.

THEOREM 6: *The operator $\mathscr{H}$ which maps pairs of convex maps on a set* C *into their basic convex homotopy on* $\mathrm{C}\times[0,1]$ *is continuous.*

PROOF: For any two given pairs of maps (f,g) and (f',g') such that

$$\|f-f'\|<\delta$$

$$\|g-g'\|<\delta$$

it follows that, if x, y, and z are points of C such that

$$x=ry+\bar{r}z \qquad (0\leq r\leq 1),$$

then

$$|rg(y)+\bar{r}f(z)-[rg'(y)+\bar{r}f'(z)]|\leq r|g(y)-g'(y)|+\bar{r}|f(z)-f'(z)|<r\delta+\bar{r}\delta=\delta.$$

From this it follows easily that

$$|H_{fg}(x,r)-H_{f'g'}(x,r)|\leq\delta.$$

3. Monotonicity Properties of the Basic Homotopy

THEOREM 7: *Let* f *and* g *be convex maps of the set* C, *and* H *the basic convex homotopy of* (f, g) *on* $\mathrm{C}\times[0,1]$. *If* $\mathrm{f}\leq\mathrm{g}$ $(\mathrm{f}\geq\mathrm{g})$ *on* C, *then* $\mathrm{H}(\mathrm{x},\cdot)$ *is monotonic increasing (decreasing) on* $[0,1]$, *with strict monotonicity holding if strict inequality holds between* f *and* g.

PROOF. Suppose $f\leq g$. By corollary 3 it is sufficient to show that

$$f(x)\leq H(x,r)\leq g(x)$$

for all $x\epsilon C$ and $0\leq r\leq 1$. Now

$$H(x,r)\leq rg(x)+\bar{r}f(x)$$

$$\leq rg(x)+\bar{r}g(x)=g(x)$$

proving half of the inequality. Also if

$$x = ry + \bar{r}z, \qquad y, z \epsilon C,$$

then

$$\begin{aligned} rg(y) + \bar{r}f(z) &\geqslant rf(y) + \bar{r}f(z) \\ &\geqslant f(ry + \bar{r}z) \\ &= f(x) \end{aligned}$$

so that

$$H(x, r) \geqslant f(x).$$

A similar proof holds if $f \geqslant g$.

To prove strict monotonicity for (say) the case $f < g$, let

$$\delta = \inf \{g(x) - f(x) : x \epsilon C\}.$$

Then $\delta > 0$, by the compactness of C. In the above argument we have

$$\begin{aligned} rg(y) + \bar{r}f(z) &\geqslant r\delta + rf(y) + \bar{r}f(z) \\ &\geqslant r\delta + f(x), \end{aligned}$$

implying $H(x, r) > f(x)$ if $r > 0$.

Next we consider monotonicity in the maps f and g by taking their domain to be a subinterval of the real line.

THEOREM 8: *Let* f *and* g *be convex maps defined on a compact subinterval* C *of the real line, and let* H *be the basic convex homotopy of* (f, g) *on* $C \times [0, 1]$. *If* f *and* g *are both monotonic increasing (decreasing) on* C, *then* $H(\cdot, r)$ *is also monotonic increasing (decreasing) on* C. *Furthermore, strict monotonicity of* f *and* g *implies strict monotonicity of* $H(\cdot, r)$.

PROOF. Consider two points (x_1, r) and (x_2, r), with $x_2 > x_1$.
If

$$x_2 = ry_2 + \bar{r}z_2$$

for some $y_2, z_2 \epsilon C$, then clearly it is possible to find y_1 and z_1 in C such that $y_1 \leqslant y_2, z_1 \leqslant z_2$, and

$$x_1 = ry_1 + \bar{r}z_1.$$

Thus

$$rg(y_2) + \bar{r}f(z_2) \geqslant rg(y_1) + \bar{r}f(z_1),$$

by the monotonicity of f and g. Since y_2 and z_2 were arbitrary, if follows that

$$\inf \{rg(y_2) + \bar{r}f(z_2) : y_2, z_2 \epsilon C, x_2 = ry_2 + \bar{r}z_2\} \geqslant \inf \{rg(y_1) + \bar{r}f(z_1) : y_1, y_2 \epsilon C, x_1 = ry_1 + \bar{r}z_1\},$$

or

$$H(x_2, r) \geqslant H(x_1, r).$$

If f and g are strictly monotonic and $x_2 - x_1 = \delta > 0$, then we note that $y_2 - y_1 \geq \delta$ or $z_2 - z_1 \geq \delta$ in the above. Now let

$$a = \inf \{f(x) - f(x-\delta) : x, x-\delta \epsilon C\}$$

$$b = \inf \{g(x) - g(x-\delta) : x, x-\delta \epsilon C\}.$$

Then $a, b > 0$, by the compactness of C and the strict monotonicity assumption, while

$$[rg(y_2) + \bar{r}f(z_2)] - [rg(y_1) + \bar{r}f(z_1)] = r[g(y_2) - g(y_1)] + \bar{r}[f(z_2) - f(z_1)] \geq \min \{rb, \bar{r}a\}.$$

Thus

$$H(x_2, r) - H(x_1, r) \geq \min \{rb, \bar{r}a\}.$$

proving strict monotonicity.

It should be noted that the fact that $f(x) \geq g(y)$ for some x and y does not imply monotonicity of a convex homotopy G of (f, g) along the line joining $(x, 0)$ and $(y, 1)$, even if the conditions of theorems 7 and 8 are satisfied. For instance, if f, g: $[0, 1] \to R$, and

$$f(x) = 1,$$

$$g(x) = x,$$

then $G(0, 0) = G(1, 1) = 1$, but clearly

$$G(\tfrac{1}{2}, \tfrac{1}{2}) \leq \tfrac{1}{2} G(0, 1) + \tfrac{1}{2} G(1, 0)$$

$$= \tfrac{1}{2}.$$

4. Specific Forms of the Basic Convex Homotopy

We have shown in theorems 2 and 4 that there are many convex homotopies connecting any given pair of convex maps. One interesting set of homotopies (because they can be written explicitly) is given in the following case. Let f and g be convex maps on C such that $f - g = a$, a constant. If h: $[0, 1] \to R$ is any convex map for which

$$h(0) = 0,$$

$$h(1) = a,$$

then the map H: $C \times [0, 1] \to R$ defined by

$$H(x, r) = f(x) + h(r)$$

is a convex homotopy of (f, g). In fact, if

$$h(r) = ra,$$

then H is the basic homotopy. This raises some questions, about the form of the basic homotopy, which will now be considered.

THEOREM 9: *Let* f *and* g *be two convex, differentiable maps on a compact subinterval* C *of the real line. If* H *is the basic homotopy of* (f, g) *on* $C \times [0, 1]$, *then a necessary and sufficient condition that*

$$H(x, r) = f(x) + r(g(x) - f(x))$$

is that f − g *is constant.*

PROOF. Consider any point $(x, \frac{1}{2})$. Then

$$H(x, \tfrac{1}{2}) = \tfrac{1}{2}f(x) + \tfrac{1}{2}g(x).$$

But if $\delta > 0$, then we must have

$$\tfrac{1}{2}H(x+\delta, 0) + \tfrac{1}{2}H(x-\delta, 1) \geq H(x, \tfrac{1}{2}),$$

or

$$\tfrac{1}{2}f(x+\delta) + \tfrac{1}{2}g(x-\delta) \geq \tfrac{1}{2}f(x) + \tfrac{1}{2}g(x).$$

Then,

$$f(x+\delta) - f(x) \geq g(x) - g(x-\delta),$$

implying

$$f'(x) \geq g'(x),$$

where f' and g' are the first derivatives of f and g, respectively. Similarly, taking $\delta < 0$, leads to

$$f'(x) \leq g'(x),$$

so that

$$f'(x) = g'(x).$$

Since x was chosen arbitrarily, this implies that $f - g$ is constant, proving necessity. Sufficiency was shown above.

THEOREM 10. *Let* f *and* g *be two convex maps on a set* C *such that, along any line segment in* C, f *and* g *are differentiable except at, at most, a finite set of points. If* H *is the basic convex homotopy of* (f, g) *on* $C \times [0, 1]$, *then a necessary and sufficient condition that*

$$H(x, r) = f(x) + r(g(x) - f(x))$$

is that f − g *is constant.*

PROOF. Consider any point $x \epsilon C$. If y is any other point of C, then by lemma 9 $f - g$ is constant on the portions of the line segment L joining x and y where f and g are both differentiable along L. By the continuity of f and g, $f - g$ is therefore constant for all points on L, since there are at most a finite number of points at which the derivative along L does not exist. Therefore,

$$f(y) - g(y) = f(x) - g(x) = a.$$

Since y was arbitrary, the theorem is proved.

Finally we show something about the explicit determination of H for certain f and g.

THEOREM 11. *Let* f *and* g *be convex maps defined on a compact interval* C *of the real line, and let* H *be the basic convex homotopy of* (f, g) *on* $C \times [0, 1]$. *For any* $(x, r) \in C \times [0, 1]$,

$$H(x, r) = rg(y) + \bar{r}f(z),$$

where y *and* z *are points in* C *for which* $x = ry + \bar{r}z$ *and* $g'(y) = f'(z)$, *if such points exist. If not, then* y *and* z *are such that* $x = ry + \bar{r}z$ *and*

$$f^-(z) \leqslant g^+(y),$$

$$g^-(y) \leqslant f^+(z),$$

where f^-, f^+, g^-, g^+ *are the left and right hand derivatives of* f *and* g, *if such points exist. If neither* of the above exist, then

$$H(x, r) = \min \{rg(y) + \bar{r}f(z): x = ry + \bar{r}z \text{ and } y \text{ or } z \text{ is an endpoint of } C\}.$$

PROOF. Let

$$h(y) = rg(y) + \bar{r}f\left(\frac{x - ry}{\bar{r}}\right)$$

for all $y \in C$ for which $(x - ry)/\bar{r} \in C$. Then $H(x, r) = \inf h(y)$. If there exists $y_0 \in C$ for which

$$f^-\left(\frac{x - ry_0}{\bar{r}}\right) \leqslant g^+(y_0)$$

and

$$g^-(y_0) \leqslant f^+\left(\frac{x - ry_0}{\bar{r}}\right),$$

then it is clear that, if $\delta > 0$,

$$h(y_0 + \delta) = rg(y_0 + \delta) + \bar{r}f\left(\frac{x - ry_0 - r\delta}{\bar{r}}\right)$$

$$\geqslant r(g(y_0) + \delta g^+(y_0))$$

$$+ \bar{r}\left(f\left(\frac{x - ry_0}{\bar{r}}\right) - \frac{r\delta}{\bar{r}} f^-\left(\frac{x - ry_0}{\bar{r}}\right)\right)$$

$$= rg(y_0) + \bar{r}f\left(\frac{x - ry_0}{\bar{r}}\right)$$

$$+ \delta r\left(g^+(y_0) - f^-\left(\frac{x - ry_0}{\bar{r}}\right)\right)$$

$$\geqslant rg(y_0) + \bar{r}f\left(\frac{x - ry_0}{\bar{r}}\right) = h(y_0),$$

whenever $h(y_0 + \delta)$ exists. (If $h(y_0 + \delta)$ does not exist, then either y_0 or $z_0 = (x - ry_0)/\bar{r}$ is an endpoint of C.) Similarly,

$$h(y_0 - \delta) \geqslant h(y_0).$$

Thus,

$$h(y_0) = \inf h(y) = H(x, r).$$

If there is no such point y_0, then for every y in the interior of C we have either

$$f^-\left(\frac{x-ry}{\bar{r}}\right) > g^+(y)$$

or

$$g^-(y) > f^+\left(\frac{x-ry}{\bar{r}}\right).$$

Thus if neither y nor $\frac{x-ry}{\bar{r}}$ is an endpoint of C, it is clear that there exists $\delta>0$ such that either

$$h(y+\delta) < h(y)$$

or

$$h(y-\delta) < h(y).$$

Since h is continuous in y and the domain of h is a closed subinterval of C, it follows that h must take its minimum value when y or $\frac{x-ry}{\bar{r}}$ is an endpoint of C. This completes the proof.

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The Powers of a Connected Graph are Highly Hamiltonian*

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Let G be a connected graph on p points. It is proved that if any k points are deleted from the graph G^{m+2}, $1 \leq m \leq p-3$ and $0 \leq k \leq m$, then the resulting graph is hamiltonian.

Key words: graph, hamiltonian, power of a graph.

Let G be a graph (finite, undirected, without loops or multiple lines). A *walk* of G is a finite alternating sequence of points and lines of G, beginning and ending with points, and where each line is incident with the two points immediately preceding and following it. A walk in which all points are distinct is called a *path*; the *length* of a path is the number of lines in it. A graph G is said to be *connected* if between any two points of G there is a path. The *distance* between two points u and v in a connected graph G is the length of a shortest path between u and v if $u \neq v$, and zero if $u = v$.

A walk with at least three distinct points in which the first and the last points are the same but all the other points are distinct is called a *cycle*. A cycle containing all the points of G is a *hamiltonian cycle* of G, and then G itself is said to be a *hamiltonian graph*. A graph G on p points is *m-hamiltonian* if the removal of any k points from G, $0 \leq k \leq m \leq p-3$, yields a hamiltonian graph (see [2]).[1]

Let G be a connected graph and $n \geq 1$. The graph G^n, called the *n*th *power of* G, has as its points those of G, and two distinct points u and v are adjacent in G^n if the distance between u and v in G is at most n.

For a connected graph G on $p \geq 3$ points, it is well known that G^3 is hamiltonian; in fact (see [1]) if x is any line of G, there is a hamiltonian cycle of G^3 which contains x. The main result of [1] was: the cube of every connected graph possessing at least 4 points is 1-hamiltonian. It is this result which we generalize as follows.

THEOREM: *If* G *is a connected graph on* p *points, then* G^{m+2} *is* m*-hamiltonian for* $1 \leq m \leq p-3$.

The proof is by construction.

To start with we make some observations. As G^3 is hamiltonian, and $G^3 \subseteq G^4 \subseteq \ldots \subseteq G^{m+2}$, it suffices to prove that the deletion of any $n \geq 1$ points from G^{n+2} yields a hamiltonian graph. Moreover, since every connected graph contains a spanning tree, without loss of generality we may assume G to be a tree. The case $m = 1$ is dealt with in [1]. So we take $m \geq 2$ for the rest of the discussion.

Let T be a tree on p points and let m be such that $2 \leq m \leq p-3$. Let $V(m) = \{u_1, u_2, \ldots, u_m\}$ be a set of m distinct points of T. Denote the unique path in T joining the points u_i and u_j of $V(m)$ by $P(u_i, u_j)$. We define the tree $\tilde{T}$ to be the subtree of T spanned by the points of all the paths $P(u_i, u_j)$, $1 \leq i, j \leq m$.

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[1] Figures in brackets indicate the literature references at the end of this paper.

For the sake of clarity we assign colors to the points of T: the points of $V(m)$ are colored *red*, those of $\tilde{T}$–$V(m)$ *green*, and the remaining points of T *blue*. Obviously every endpoint of $\tilde{T}$ is red. Designate one of the endpoints of the nontrivial tree $\tilde{T}$ as the *initial* point. The remaining endpoints of $\tilde{T}$ will be referred to as *reversing* points. For a point u of $\tilde{T}$ we denote by $d(u)$ and $\tilde{d}(u)$, the degree of u in T and $\tilde{T}$ respectively. If $\tilde{d}(u) \geq 3$, then u will be called a *crucial* point, and this may be red or green.

The $n(\geq m)$ points of $\tilde{T}$ are labeled 1, 2, . . ., n in the following manner (see fig. 1). The initial point of $\tilde{T}$ is labeled 1. The unique point of $\tilde{T}$ adjacent to the initial point is labeled 2. Suppose that the labels 1, 2, . . ., i have been assigned, $1 < i \leq n$. If $\tilde{d}(i) \geq 3$, i.e., if i is a crucial point, then a point of $\tilde{T}$ adjacent to i and not already labeled is designated $i+1$. If $\tilde{d}(i) = 2$, then the unique nonlabeled point of T adjacent to i is labeled $i+1$. If $\tilde{d}(i) = 1$, then i is a reversing point. If there are no crucial points on the path in $\tilde{T}$ between 1 and i, then $\tilde{T}$ itself is a path, and it follows that $i = n$. If not, let $S(i) = (j_1, j_2, \ldots, j_{r_i})$ be the sequence of all the crucial points between 1 and i, and such that $1 < j_1 < j_2 < \ldots < j_{r_i} < i$. If there is a nonlabeled point of $\tilde{T}$ adjacent to j_{r_i}, then we label it $i+1$. If not, we consider the nonlabeled points of $\tilde{T}$ adjacent to j_{r_i-1}, j_{r_i-2}, and so on till j_1. If even j_1 has all the points adjacent to it in $\tilde{T}$ already labeled, then clearly $i = n$.

As already noted, if $\tilde{T}$ has at least one crucial point, then with every reversing point i of $\tilde{T}$ we can associate a unique *crucial sequence* $S(i)$ as defined above. If $\tilde{T}$ is a path, write $S(n) = \emptyset$. Moreover, if j is a crucial point, then there are at least $\tilde{d}(j) - 1$ reversing points whose associated crucial sequences contain j. (See fig. 1.).

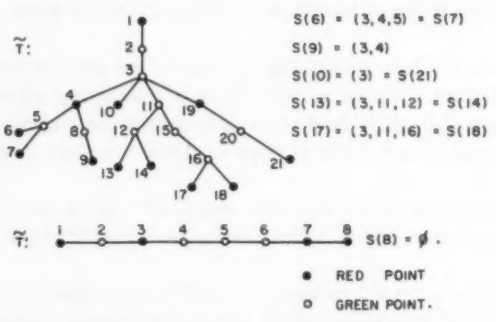

FIGURE 1. *Examples of trees* $\tilde{T}$; *their labeling and crucial sequences.*

Every point i of $\tilde{T}$ is adjacent to $d_i = d(i) - \tilde{d}(i) \geq 0$ blue points of T. Let the forest in $T - i$ to which these d_i points belong be denoted F_i. For the sake of completeness, if $d_i = 0$, we will reflect this by writing $F_i = \emptyset$. If $d_i \geq 1$, let the d_i components of F_i be the trees T_t on p_t points, $1 \leq t \leq d_i$. (See fig. 2.) Let x_t be the point in T_t which is adjacent to i, and x_t' a point in T_t which is adjacent to x_t (if $p_t = 1$, we assign a second label x_t' to x_t). Since $m \geq 2$, the set of points $\{x_t, x_t' | 1 \leq t \leq d_i\}$ induce a complete graph in T^{m+2}.

Consider the graph $T_t^3 \subseteq T^{m+2}$. We have

(i) if $p_t \geq 3$, then by earlier remarks there exists a hamiltonian cycle in T_t^3 containing the line $x_t x_t'$, and by deleting this line from this cycle there results a spanning path P_t in T_t^3 such that x_t and x_t' are the endpoints of P_t,

(ii) if $p_t = 2$, T_t is itself the path P_t, and

(iii) for $p_t = 1$, $x_t = T_t = P_t$.

It is now possible to construct a special path $P(i)$ in T^{m+2} which spans F_i. Define

$$P(i) = \begin{cases} x_1 P_1 x_1' \quad \text{or} \quad x_1' P_1 x_1, & \text{if} \quad d_i = 1 \\ x_1 P_1 x_1' x_2 P_2 x_2' x_3 \ldots\ldots x_{d_i-1} P_{d_i-1} x_{d_i-1}' x_{d_i}' P_{d_i} x_{d_i}, & \text{if} \quad d_i \geq 2, \end{cases}$$

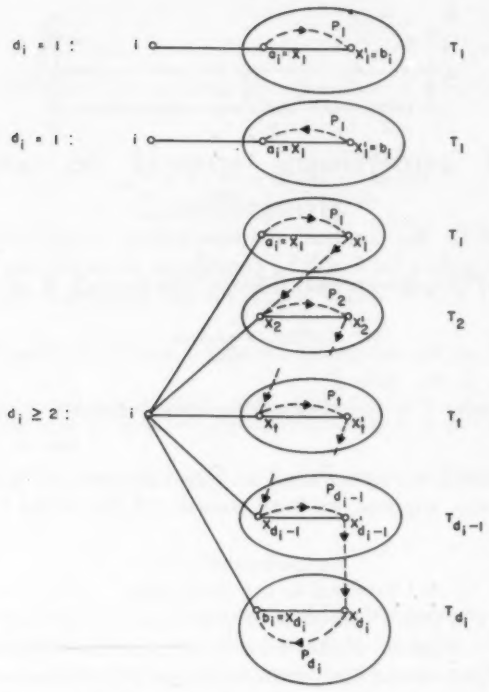

FIGURE 2. *The forest* F_i *and its spanning path.*

where $x_kP_kx_k'$ refers to the path P_k starting at x_k and ending at x_k' (similarly for $x_k'P_kx_k$). If $F_i \neq \emptyset$, we are only concerned with the starting and ending points of the spanning path $P(i)$ of F_i. Towards this end we set

$$a_i = x_1$$

and

$$b_i = \begin{cases} x_1' & \text{if} \quad d_i = 1 \\ x_{d_i} & \text{if} \quad d_i \geq 2. \end{cases}$$

Then $P(i;\ a_i,\ b_i)$ will denote the path $P(i)$ starting at a_i and ending at b_i; whereas $P(i;\ b_i,\ a_i)$ will be the path $P(i)$ beginning at b_i and ending at a_i.

We now construct a hamiltonian cycle C in $T^{m+2} - V(m)$. First, an outline will be suggested. Starting at the initial point 1, we move around the points of the tree $\bar{T}$ in the order of its labeling. At each point i with $F_i \neq \emptyset$, the spanning path $P(i;\ a_i,\ b_i)$ or $P(i;\ b_i,\ a_i)$ of F_i is included in C in a specific order. For green points of $\bar{T}$ having $F_i = \emptyset$, a special procedure is adopted. Picking on C the first such green point encountered, the remaining are picked alternately while going towards a reversing point. Those missed, as well as the green points with $F_i \neq \emptyset$, are picked up while returning (through crucial points) from a reversing point to the next point of $\bar{T}$ in its labeling. The residual green points are picked while going from the last reversing point n to the starting point of C. Clearly, C contains all the nonred points of T, and is in fact a cycle. Also, the adjacencies in T^{m+2} are used to proceed from the considerations at the ith stage to the next.

First we settle the only extreme case. Suppose that $\bar{T}_0$ is a path on $n = m+1$ points, $d_1 = d_n = 1$, and $F_i = \emptyset$ for $2 \leq i \leq n-1$ (see fig. 3). Let g denote the only green point of $\bar{T}_0$. Then

$$C = \underline{P(1;\ a_1,\ b_1)gP(n;\ b_n,\ a_n)a_1}.$$

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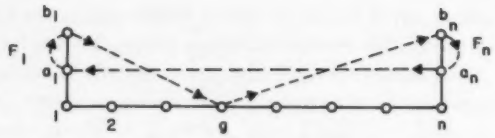

FIGURE 3. $\bar{T}_0$ *with* $n = m+1$, $d_1 = d_n = 1$.

Now suppose that $\bar{T} \neq \bar{T}_0$. We construct the hamiltonian cycle C as follows, keeping in mind that the first point that is picked on C will be considered as its starting point.

Step 1: Consider $1 \in \bar{T}$. If $F_1 \neq \emptyset$, pick $P(1; a_1, b_1)$ and proceed to the next step. If $F_1 = \emptyset$, we go to step 2.

Step 2: $F_2 \neq \emptyset$: Pick $P(2; a_2, b_2)$ and proceed to step 3. For $n = 2$, either $\underline{P(1; a_1, b_1)P(2; a_2, b_2)a_1}$ or $\underline{P(2; a_2, b_2)a_2}$ is the cycle C.

$F_2 = \emptyset$ and the point 2 is red: Proceed to step 3 directly. If $n = 2$, then $\underline{P(1; a_1, b_1)a_1}$ is C.

$F_2 = \emptyset$ and the point 2 is green: Pick 2 on C and proceed to the next step.

Continuing this process, suppose we have considered the points 1, 2, . . ., $i-1$, i.e., *step* $i-1$ has been taken.

Step i: Suppose $\bar{d}(i) \geq 2$.

$F_i \neq \emptyset$: Pick $P(i; a_i, b_i)$ and proceed to the next step.

$F_i = \emptyset$ and the point i is red: Proceed to step $i+1$.

$F_i = \emptyset$ and the point i is green: Pick i on C if an immediately preceding green point j with $F_j = \emptyset$ has not been picked and then move to step $i+1$, otherwise go to step $i+1$ directly.

Suppose $\bar{d}(i) = 1$.

Here i is a reversing point.

Let $i \neq n$. If $F_i \neq \emptyset$, pick $P(i; a_i, b_i)$ (if $F_i = \emptyset$, this is absent) and pick up in reverse succession all the unpicked green points on the path in $\bar{T}$ between the points i and $i+1$.

Let $i = n$. If $F_n \neq \emptyset$, pick $P(n; a_n, b_n)$ (if $F_n = \emptyset$, this is absent) and pick up on C, all the remaining green points in reverse succession towards 1, and reach the starting point of C.

This completes the construction.

The result proved above is the best possible in the sense that the graph G^{m+2} is not necessarily $(m+1)$-hamiltonian. For example, let P be a path on $m+4$ points, $m \geq 1$. Let $V(m+1)$ be any set of $m+1$ points of P, excluding the end points. Then the graph $P^{m+2} - V(m+1)$ is a path on 3 points and clearly nonhamiltonian. On the other hand, if G is a connected graph on $p \geq 3$ points, then G^n is the complete graph K_p for all $n \geq p-1$, and hence it is always $(p-3)$-hamiltonian (see [2]).

The theorem does not hold for $m = 0$, i.e., the square of a connected graph need not be hamiltonian. But if *connected* is replaced by *block*, the proposition reads—*the square of a block on 3 or more points is hamiltonian.* M. D. Plummer has conjectured that this is true.

Added in proof. H. Fleishner has confirmed Plummer's conjecture.

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Exact Solutions of Linear Equations With Rational Coefficients*

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Improvements of a congruential method for finding the exact solutions of systems of linear equations with rational coefficients are described. Typical execution times on the CDC 1604–A are given, as well as the Fortran program.

Key words: Congruences; exact solutions; linear equations; modular arithmetic.

1. Introduction

An algorithm for computing the exact solutions of linear equations with rational coefficients, and its computer implementation, were described in [1].[1] The basic idea of the algorithm is to convert the original system of equations into a system of congruences modulo various primes p_i, and combining the solutions by a procedure suggested by the Chinese Remainder Theorem. This process is continued until the sequence of solutions modulo $p_1p_2 \ldots p_k$, $k=1, 2, \ldots$ converges to the true solution. The major part of the computation is performed in single precision. See also Newman [4] who used the method for computing the inverses of ill-conditioned matrices, and Knuth [3, p. 256], who remarked that for ill-conditioned matrices the procedure "gives a method for obtaining the *true* answers in less time than any known method can produce reliable *approximate* answers!"

Our program provides for a final substitution check for verifying convergence, i.e., verifying that the computed values satisfy the original system. It is applied after two successive iterations produce no change in the solution vectors. If so implemented, and assuming sufficient memory space, the method produces the exact solution space for *any* solvable linear system with rational coefficients. Moreover, the algorithm is effective, in the sense that the exact solution space is produced within a reasonable time for systems that are not too large. It cannot end up with a wrong or no solution, as additional iterations are made should the substitution check fail.

The implementation of the algorithm has since been improved. As a result, the computation of the 9 independent exact solutions of a system of 111 homogeneous equations in 120 unknowns of rank 111 with integral coefficients in the range $[-2180, 2568]$ which took 60 min on a CDC 1604–A by the old method, now takes only 19 min on the same computer. The program is still in the form of standard Fortran subroutines, and no pains were taken to write a particularly economic program.

In the sequel it is assumed that the reader is reasonably familiar with the essential features of [1].

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[1] Figures in brackets indicate the literature references at the end of this paper.

2. The Improvements

There are four main improvements: Use of larger primes; using the Cantor representation for constructing the solution mod $p_1p_2 \ldots p_k$ after the kth iteration (by the Chinese Remainder Theorem); a logical simplification in determining whether to retain or discard a new prime; and using a faster algorithm for finding the greatest common divisor (g.c.d.) of the components of any solution vector. These improvements will now be described one for one.

(i) *Use of larger primes.* In [1], primes of the order of 10^7, just less than half the machine word length, were employed. Primes of the order of 10^{14}, just less than one machine word are now used. Such primes were supplied to us through the courtesy of Herschel F. Smith from IBM. This saves about half the number of iterations (primes). In the above example, it reduced the number of iterations from six to four. Of course, we could have used the squares of primes of the order of 10^7 to obtain the same effect. However, the probability that a prime divides any of the principal minors of a matrix decreases with the size of the prime. Hence it is of some advantage to use the largest primes just less than a machine word.

(ii) *Use of the Cantor representation.* Let $m_1, \ldots, m_s$ be odd positive integers, relatively prime in pairs. Any number N in the range

$$\left[-\frac{m_1m_2 \ldots m_s}{2}\right] < N \leqslant \left[\frac{m_1m_2 \ldots m_s}{2}\right]$$

is uniquely representable by the *Cantor representation*, also referred to, by several authors, as the *mixed radix representation:*

$$N = a_1 + a_2m_1 + a_3m_1m_2 + \ldots + a_sm_1m_2 \ldots m_{s-1},$$

where

$$\left[-\frac{m_i}{2}\right] < a_i \leqslant \left[\frac{m_i}{2}\right], \qquad i = 1, 2, \ldots, s.$$

The Cantor representation of a number given by its residues mod m_i, $i = 1, 2, \ldots, s$, can be determined by computations in which all numbers occurring have absolute value not exceeding max m_i, in the present case single precision. See e.g., [2]. The solution check of [1] is now performed when for any fixed k, $a_k = 0$ for all components of the solution vectors.

Thus, the main computation of the solution vectors is now performed in single precision, resulting in a large time saving. Multiple precision is required only in the final conversion of the Cantor representation to decimal representation, and in the—optional—subsequent computation of the g.c.d. of the components of each solution vector.

(iii) *A logical simplification.* On pp. 110–111 of [1], a method was described which guarantees that each triangularization converges to the *same* largest nonsingular submatrix of the coefficient matrix A. For this, a lexicographic ordering of rows and columns of A had to be checked. This has now been changed as follows: The triangularization of A (mod p_1) induces a certain interchange of rows and columns in A. If ρ is the rank of A mod p_1, let $i_1, \ldots, i_\rho, j_1, \ldots, j_\rho$ be the rows and columns of A appearing in the triangularized principal submatrix of order ρ. The rows and columns of A itself are now reordered, so that $i_1, \ldots, i_\rho, j_1, \ldots, j_\rho$ appear as its first ρ rows and columns. Call this permuted matrix B. In each subsequent iteration mod p_i $(i > 1)$, the triangularization is performed without changing any of the first ρ rows and columns in B. In the triangularized matrix, denote by ρ_i the order of the largest nonsingular principal submatrix. If $\rho_i < \rho$, p_i must be discarded; if $\rho_i > \rho$, the primes $p_1, \ldots, p_{i-1}$ must be discarded and a new matrix B with a greater rank is formed from A; if $\rho_i = \rho$, which is the normal case, the solution mod p_i is used to determine the coefficients a_i of the Cantor representation of all components of the solution vectors.

This modification does not save much time. In practice it only saves logical operations and manipulations, as it almost never happens that a given large prime divides a nonzero principal minor. However, the logical simplification results in a more compact and elegant program.

(iv) *Computation of the g.c.d.* The last step in [1] was to find the g.c.d. of the components of each of the solution basis vectors and to divide them out, so as to obtain *primitive* solutions, i.e., solutions such that the g.c.d. of the components of each solution vector is unity. Instead of computing the g.c.d. by the Euclidean Algorithm, i.e., by a series of multiple precision divisions, it is found by a series of shifts, using an economic algorithm of Stein [5], which, according to Knuth [3, p. 297], was previously given by Silver and Terzian:

Let t be any positive integer stored in binary form in a computer register. The highest power of 2 dividing t can easily be determined by shifting t to the right until its least significant nonzero bit is located in the least significant position of the register. This results in an odd integer $t' = 2^{-k}t$. We shall designate this operation by *shift*, i.e., $t' = \text{shift}(t)$.

Let a, b be two positive integers, and let

$$a_0 = \text{shift } (a) = 2^{-k}a, \qquad b_0 = \text{shift } (b) = 2^{-l}b.$$

Let $m = \min(k, l)$. The algorithm now proceeds as follows:

$$\begin{aligned} a_1 &= \text{shift } |a_0 - b_0|, & b_1 &= \min(a_0, b_0) \\ a_2 &= \text{shift } |a_1 - b_1|, & b_2 &= \min(a_1, b_1) \\ &\cdot \\ &\cdot \\ &\cdot \\ a_n &= \text{shift } |a_{n-1} - b_{n-1}|, & b_n &= \min(a_{n-1}, b_{n-1}) \\ a_{n+1} &= \text{shift } |a_n - b_n|. \end{aligned}$$

The procedure terminates when $a_n = b_n$, and then $(a, b) = 2^m a_n$.

In our example, a multiple precision g.c.d. was obtained for each of the 9 solution vectors. The computation of these g.c.d. and dividing them out now takes 2.5 min instead of the previous 7.5 min.

Finally, we should remark that the substitution check, which is also a multiple-precision operation, takes 6 min for our example. It is extremely rare that a substitution check fails when large primes are used, and therefore it seems reasonable to dispose of it in general. In fact, no substitution check is normally made in any of the conventional iterative schemes for solving linear equations—including those for which convergence is not guaranteed a priori even when the system is known to be solvable.

On the other hand, it is easy to fabricate a failing case. For simplicity assume that there is only one solution vector $V = (v_1, v_2, \ldots, v_t)$, whose Cantor representation is

$$v_i = a_{i1} + a_{i2}p_1 + a_{i3}p_1p_2 + \ldots + a_{ik}p_1p_2 \ldots p_{k-1} + \ldots + a_{is}p_1p_2 \ldots p_{s-1}, \quad 1 \leq i \leq t,$$

where $p_1, p_2, \ldots$ are distinct primes. For obtaining a failing case, we simply choose $a_{ik} = 0$, $1 \leq i \leq t$, and a_{ij}, $j \neq k$ arbitrarily, with the only condition that $a_{il} \neq 0$ for some $l > k$ and for some i.

A vector V of this form can clearly also be characterized as follows. Suppose that $V^{k-1} = (v_1^{k-1}, v_2^{k-1}, \ldots, v_t^{k-1})$ is the solution mod $p_1p_2 \ldots p_{k-1}$, i.e.,

$$v_i \equiv v_i^{k-1} (\text{mod } p_1p_2 \ldots p_{k-1}), \qquad 1 \leq i \leq t.$$

Then

$$a_{ik} = 0,\ 1 \leq i \leq t,\ a_{il} \neq 0,\ l > k \qquad \text{for some } i$$

if and only if

$$v_i \equiv v_i^{k-1} (\text{mod } p_k),\ 1 \leq i \leq t,\ v_i \neq v_i^{k-1} \qquad \text{for some } i.$$

Disposing of the substitution check and the g.c.d. computation, solution time in our example

reduces to 10 min. By comparison, the approximate computation of a *well-conditioned* 111×111 system by standard numerical floating number techniques takes about 3 min on the CDC 1604–A.

3. Machine Program

The program given below is the full version, i.e., it includes computation of the g.c.d. and the substitution check imbedded in the program "Solve." The matrix of the homogeneous equations coefficients is read into the computer from magnetic tape no. 1. Other data to the program is provided by three data cards. The first card contains three numbers: the number of rows and columns of the matrix, and the number of primes supplied. The second and third cards contain the supplied primes.

Functions used in this program are:

"Inv"—computes the inverse of an integer t mod p which is required for solving the system mod p.

"Irem"—IREM(t_1, t_2, p) outputs an integer t satisfying $t \equiv t_1 t_2 (\mathrm{mod}\ p)$, $-p < t < p$. Since the product $t_1 t_2$ is normally a double precision number, this routine is written in machine language.

"Shift"—shifts a multiple-precision number to the right k positions until a binary 1 appears at the least significant position. On its left, k binary zeros are shifted in. Because of its multiple-precision character, this routine is also written in machine language. In the program listed below it appears directly after "Irem," before "Setpreci."

"Mod"—MOD (t, p) transforms the single-precision integer t obtained as a result of an addition or subtraction of two numbers x_i, $-(p-1)/2 \leq x_i \leq (p-1)/2$, $i = 1, 2$, or of an IREM operation, to an integer t' satisfying $t' \equiv t (\mathrm{mod}\ p)$ and $-(p-1)/2 \leq t' \leq (p-1)/2$.

"Setpreci"—A Fortran subroutine which controls the multi-precision package which is written in machine language. Because this package is in a binary deck form, it is not included in the program listed below. Functions used from this package are: "If(Itest(t))"—for checking if a multiple precision integer t is negative zero or positive; "Multout"—for printing a multiple precision integer.

```
      PROGRAM SOLVE
      COMMON M1,M2,NZ,M,N,KP,KQ,KI,MA(111,120),IZ(120),NEW(9,9),
     1 NT(4,120),KT(20),IY(120),JSOL(120),KSOL(120),JS(112,9,6),KG(8)
     2 ,KE(8),KF(8),KO(8),NA(6),NB(6),NC(6),ND(6)
      TYPE MULTIPL6(6) A,B,C,KG,D,GCD,KC ,KSOL
      COMMON/SHIFTS/KK
      EQUIVALENCE (A,NA),(B,NB),(C,NC),(D,ND)
      READ 55,M,N,NZ
      READ 797,(KT(I),I=1,nz)
      REWIND 1 $ DO 987 I=1,M
  987 READ TAPE 1,(MA(I,J),J=1,N)
      PRINT 7,M,N,NZ $ DO 63 I=1,M
   63 IY(I)=I $ KR=0 $ PRINT 2,(KT(I),I=1,NZ) $ DO 94 J=1,N
   94 IZ(J)=J $ DO 200 L=1,NZ $ KP=KT(L) $ KQ=KP/2. $ KD=MK=1
      DO 75 I=1,M$DO 75 J=1,N$IS=MA(I,J)-(MA(I,J)/KP)*KP$ IF(IS)76,75,75
   76 IS=KP+IS
   75 MA(I,J)=IS
   23 DO 122 K=MK,KR $ IF(IT.EQ.1)10,43
    8 PRINT 88,KP $ MS=1 $ GO TO 201
   43 I1=IY(K) $ J1=IZ(K) $ KK=MA(I1,J1)
   10 MK=MK+1 $ IF(KK-1)8,33,34
   34 KD=IREM(KD,KK,KP) $ IM=INV(KK,KP) $ DO 32 JL=MK,N $ J2=IZ(JL)
   32 MA (I1,J2)=IREM(MA(I1,J2),IM,KP)
```

```
 33 DO 122 I = MK,M $ I2 = IY(I) $ IL = MA(I2,J1) $ IF(IL.EQ.0)122,31
 31 DO1J = MK,N$J2 = IZ(J)$IS = MA(I2,J2) - IREM(MA(I1,J2),IL,KP)$IF(IS)72,1,1
 72 IS = KP + IS
  1 MA(I2,J2) = IS
122 CONTINUE
    DO6I = MK,M$I1 = IY(I)$DO6J = MK,N$J1 = IZ(J)$KK = MA(I1,J1)$IF(KK.EQ.0)6,5
  5 KR = MK$IT = 1$IY(I) = IY(KR)$IY(KR) = I1$IZ(J) = IZ(KR)$IZ(KR) = J1$GOTO23
  6 CONTINUE $ IW = IT - 1 $ KF(IT) = KP $ IS = 1 $ KE(1) = 1 $ DO 70 I = 1,IW
    I1 = I + 1 $ IS = IREM(IS,KF(I),KP)
 70 KE(I1) = IS
    PRINT 51,KP,KD,IT $ IF(IT.EQ.1)47,29
 29 IS = KE(IT) $ IV = INV(IS,KP) $ NU = 0 $ DO 944 KL = 1,IW
    KS = IREM(KO(KL),KE(KL),KP) $ IF(KS)971,979,979
971 KS = KP + KS
979 NU = NU + KS $ IF(NU - KP)944,974,974
974 NU = NU - KP
944 CONTINUE $ IS = KD - NU $ MS = KO(IT) = MOD(IREM(IS,IV,KP)) $ GO TO 95
 47 MS = 1 $ KO(1) = MOD(KD) $ KI = N - KR $ PRINT 56,KR,KI,(IY(I),I = 1,M)
    PRINT 58,(IZ(J),J = 1,N)
 95 DO 26K=1,KI$DO26I=1,KR$I1=I-1$K1=KR-I1$MX=0$DO38J=1,I1$K2=MK-J
    MX = MX - IREM(JSOL(K2),MA(IY(K1),IZ(K2)),KP) $ IF(MX)78,38,38
 78 MX = MX + KP
 38 CONTINUE$IS = MX - IREM(KD,MA(IY(K1),IZ(KR + K)),KP)$IF(IS)37,27,27
 37 IS = IS + KP
 27 JSOL(K1) = IS $ IF(IT.EQ.1)28,90
 28 JS(K1,K,1) = MOD(IS) $ GO TO 26
 90 NU=0 $DO44 KL=1,IW $ KS=IREM(JS(K1,K,KL),KE(KL),KP)$IF(KS)71,79,79
 71 KS = KP + KS
 79 NU = NU + KS $ IF(NU - KP)44,74,74
 74 NU = NU - KP
 44 CONTINUE $ JS(K1,K,IT) = 0 $ IS = IS - NU $ IF(IS.EQ.0)26,45
 45 MS = 1 $ JS(K1,K,IT) = MOD(IREM(IS,IV,KP))
 26 CONTINUE $ IT = IT + 1
201 REWIND 1 $ DO 202 I = 1,M $ READ TAPE 1,(MA(I,J),J = 1,N)
202 CONTINUE $ IF(MS.EQ.0)203,200
200 CONTINUE $ GO TO 80
203 PRINT 153
    KG(1) = 1 $ DO 710 I = 2,IW
710 KG(I) = KG(I - 1)*KF(I - 1)
    KC = KO(1) $ DO 720 I = 2,IW
720 KC = KC + KO(I)*KG(I)
    C = KC $ IV = 7 - IW $ IF(ITEST(C))751,80,752
751 C = - C
752 CALL SHIFT(NC(IV),IW) $ I5 = KK
    DO 49 J = 1,KI $ NOS = I5 $ A = C $ PRINT 100,J
    DO 50 I = 1,KI $ KSOL(KR + I) = 0
 50 CONTINUE $ KSOL(KR + J) = KC
    DO 40 I = 1,KR $ B = JS(I,J,1) $ JSOL(I) = 1 $ DO 42 K = 2,IW
 42 B = B + JS(I,J,K)*KG(K)
    CALL MULTOUT(B,51)
    KSOL(I) = B
    IF(ITEST(B))715,716,717
```

```
716 JSOL(I)=0 $ GO TO 40
715 B=-B $ JSOL(I)=-1
717 DO 718 K=1,IW $ I1=7-K
718 JS(I,J,K)=NB(I1) $ CALL SHIFT(NB(IV),IW) $ IF(KK.GE.NOS)721,722
722 NOS=KK
721 D=A-B
    IF(ITEST(D))725,40,724
725 D=-D
724 CALL SHIFT(ND(IV),IW) $ A=B $ B=D $ GO TO 721
 40 CONTINUE $ GCD=A*2**NOS
    PRINT 669
    CALL MULTOUT(GCD,51)
    DO 730 I=1,KR $ IF(JSOL(I).EQ.0)730,731
731 DO 732 K=1,IW $ I1=7-K
732 ND(I1)=JS(I,J,K) $ NV=D=D/GCD $ J2=IZ(I) $ IF(JSOL(I).EQ.1)733,734
734 NV=-NV
733 PRINT 538,(NT(K,J2),K=1,M1)
    PRINT 539,NV
730 CONTINUE $ J2=IZ(KR+J) $ NV=KC/GCD
    PRINT 538,(NT(K,J2),K=1,M1)
    PRINT 539,NV
    DO 61 I=1,M $ A=0 $ DO 52 JL=1,N
 52 A=A+KSOL(JL)*MA(I,IZ(JL)) $ IF(ITEST(A))82,61,82
 82 PRINT 53,J,I
 61 CONTINUE
 49 CONTINUE
  2 FORMAT(/50X,8H PRIMES.,//(I14,2X))
  7 FORMAT(1H1,3H M=,I3,3H N=,I3,4H NZ=,I3,//,20X,7H MATRIX,//)
 51 FORMAT(1H1,50X6HPRIME=,I14/I50,12H=DETERMINANT/I50,11H
                                                    ITERATIONS)
 53 FORMAT(1H1,20X,8H NOT YET,20X,2I20)
 55 FORMAT(23I5)
 56 FORMAT(//20X,11HFIRST PRIME,5X,5HRANK=,I3,5X,8HNULLITY=,I3//40X,14
   1HORDER OF LINES,//(23Iff))
 58 FORMAT(//,40X,16HORDER OF COLUMNS,//(23I5))
 88 FORMAT(50XI14,23H THIS PRIME WAS DROPPED)
100 FORMAT(1H1,//50X,I3///)
153 FORMAT(/,20X,32HCONVERGENCE OBTAINED AND CHECKED,//)
538 FORMAT(/,20X,10I3)
539 FORMAT(I20, 8HX1 X2 X3,//)
669 FORMAT(1H1,//50X,6H G.C.D//)
797 FORMAT(5(I14,2X))
 80 RETURN $ END
    FUNCTION INV(KX,KP)
    K1=KP $ K2=KX $ M1=0 $ M2=1 $ IF(K2-1)2,4,5
  4 INV=K2 $ RETURN
  6 M1=M2 $ M2=M3 $ K1=K2 $ K2=K3
  5 IQ=K1/K2 $ M3=M1-M2*IQ $ K3=K1-K2*IQ $ IF(K3-1)2,7,6
  7 K2=M3-(M3/KP)*KP $ IF(K2)8,2,4
  8 K2=K2+KP $ GO TO 4
  2 INV=0
    END
```

```
      FUNCTION MOD(IX)
      COMMON M1,M2,M3,M4,M5,KP,KQ
      IF(IX)1,2,3
    2 MOD=IX $ RETURN
    1 IF(KQ+IX)4,2,2
    4 MOD=KP+IX $ RETURN
    3 IF(KQ-IX)5,2,2
    5 MOD=IX-KP
      END
          IDENT          IREM
          ENTRY          IREM
IREM      SLJ            **
          SIU       1    IR3
          LIU       1    *-1
          SIL       1    IR1
          INI       1    1
          SIL       1    IR2
          INI       1    1
IR1       SIL       1    IR3
          LIU       1    **
          LDA       1
          LIL       7    IR1
IR2       MUI       1
          LIU       1    **
          DVI       1
          LLS            48
IR3       ENI       1    **
          SLJ            **
          END
          IDENT          SHIFT
          ENTRY          SHIFT
SHIFTS    BLOCK
          COMMON         NSHIFT
SHIFT     SLJ            **
          SIU       1    EX
          SIL       2    EX
          LIU       1    SHIFT
          ENA
          STA            =SNZ
          LDA       1
          SAL            N
          ARS            24
          INI       1    1
N         SIU       1    EX+2
          LIL       1    **
          INI       1    -1
          SAL            BEGIN
          SAL            CHANGE
          SAL            LOOP
          INA            1
          SAU            STORE
BEGIN     ENI       2
```

```
            LDA     1  **
            AJP        ZERO
            ENQ
SH          LRS        1
            QJP     M  NEG
            INI     2  1
            SLJ        SH
NEG         LLS        1
            ENQ     2
            STQ        NSHIFT
            QJP        EX
            IJP     1  LOOP
EXIT        STA     7  BEGIN
EX          ENI     1  **
            ENI     2  **
            LDA        NZ
            RAD        NSHIFT
            SLJ        **
LOOP        STA        =ST
            LDA     1  **
            ENQ
            LRS     2
            STA        =ST1
            QRS        1
            LDA        T
            ADL        =O3777777777777777
STORE       STA     1  **
            LDA        T1
            IJP     1  LOOP
            SLJ        EXIT
ZERO        SIL     1  =SNN
ZERO1       INI     2  47
            IJP     1  CONT
            ENA        -1
            STA        NSHIFT
            SLJ        EX
CONT        LDA     7  BEGIN
            AJP        ZERO1
            SIL     2  =SNZ
            LIL     2  NN
CHANGE      LDA     7  BEGIN
            STA     2  **
            INI     2  -1
            IJP     1  CHANGE
            ENA
+           STA     7  CHANGE
            IJP     2  *
            LIL     1  NN
            SLJ        BEGIN
            END
      SUBROUTINE SETPRECI(NUM,LOG)
      COMMON / MULTINCM / N,IA(50),IC(50),ID(50)
```

```
      DATA (N=6)
      RETURN
      ENTRY ERR2
      PRINT 100,NUM,LOG
  100 FORMAT (46H ERROR IN ADDITION TYPE OVER-FLOW CALL FROM
     1,O16, ,18H FIRST LOCATION ,O16)
      STOP
      ENTRY ERR1
      PRINT 101,NUM,LOG
  101 FORMAT (49H ERROR IN DIVISION TYPE ZERO-DIVISOR CALL
     1FROM ,O16, ,16H FIRST LOCATION ,O16 )
      STOP
      ENTRY PRINTOUT
      WRITE (NUM,102) (ID(K),K=1,N)
  102 FORMAT (5X,5(I14,X))
      END
     DATA
   111   120     10
7908189600581  7908189600583  7908189600587  7908189600589  7908189600593
7908189600599  7908189600601  7908189600607  7908189600611  7908189600613
```

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An Improvement of the Fischer Inequality

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(October 21, 1970)

An improvement of the classical Fischer inequality for the determinant of a positive definite hermitian matrix is proved. It is used to analyze the Hadamard determinant theorem.

Key words: Fischer inequality; Hadamard determinant theorem; permanent; positive definite hermitian matrix.

1. Introduction

Let $H = (h_{ij})$ be an n-square positive semidefinite hermitian matrix, $n \geq 2$. The justly famous Hadamard determinant theorem [3; 1, p. 64; 5, p. 114][1] states that

$$\prod_{t=1}^{n} h_{tt} \geq \det H.$$

Two of the many generalizations of this theorem are of interest to us.

Partition H,

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^{*} & H_{22} \end{bmatrix} \tag{1}$$

so that H_{22} is k square. E. Fischer [2; 5, p. 117–118] proved that

$$\det H_{11} \det H_{22} \geq \det H.$$

One obtains Hadamard's theorem from Fischer's by induction.

In 1918, I. Schur [7] extended Fischer's inequality. He defined certain matrix functions: Let G be a subgroup of the symmetric group S_n. Suppose λ is a character of degree s on G. Then

$$d(H) \equiv \sum_{\sigma \in G} \lambda(\sigma) \prod_{t=1}^{n} h_{t\sigma(t)}.$$

If $G = S_n$ and $\lambda = \text{sgn}$, $d = \det$. If $G = S_n$ and $\lambda \equiv 1$, $d = \text{per}$ (permanent). Finally, if $G = \{1\}$ then $d(H) = s \prod_{t=1}^{n} h_{tt}$. Schur proved that

$$d(H) \geq s \det (H).$$

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[1] Figures in brackets indicate the literature references at the end of this paper.

If S'_k is the symmetric group on $\{n-k+1, \ldots, n\}$, $G=S_{n-k}\times S'_k$, and $\lambda=\text{sgn}$, one obtains Fischer's inequality.

In this note an inequality improving Fischer's is derived. Though the methods are simple, the result allows a sharp analysis of Hadamard's theorem.

2. Results

THEOREM 1: *Let* H *be a positive definite hermitian matrix partitioned as in* (1). *Then*

$$\det \mathrm{H}_{11} \det \mathrm{H}_{22} - \det \mathrm{H} \geq \det \mathrm{H}_{11} \det (\mathrm{H}_{12}^* \mathrm{H}_{11}^{-1} \mathrm{H}_{12})$$

with equality when $\mathrm{k}=1$.

When $n=2k$, the result becomes

$$\det H_{11} \det H_{22} - \det H_{12}^* \det H_{12} \geq \det H,$$

a special case of Schur's theorem.

Before proving Theorem 1, we introduce the *Schur complement* of H_{11} in H as

$$(H/H_{11}) \equiv H_{22} - H_{12}^* H_{11}^{-1} H_{12}.$$

LEMMA (known): *If* H *is positive definite hermitian, so is* $(\mathrm{H}/\mathrm{H}_{11})$; *and* $\det \mathrm{H} = \det \mathrm{H}_{11} \det (\mathrm{H}/\mathrm{H}_{11})$.

PROOF: Haynsworth [4] has noticed that

$$Q^*HQ = \begin{bmatrix} H_{11} & 0 \\ 0 & (H/H_{11}) \end{bmatrix} \text{ where } Q = \begin{bmatrix} I_{n-k} & -H^{-1}H_{12} \\ 0 & I_k \end{bmatrix}.$$

Hence, (H/H_{11}) is positive definite because the nonsingular congruence, Q^*HQ, preserves positive definiteness. The determinant formula (due originally to Schur) follows because $\det Q = 1$.

PROOF of THEOREM 1: It is a well known and elementary fact that if A and B are positive semidefinite hermitian matrices of the same size then

$$\det (A+B) \geq \det A + \det B.$$

(In fact, a much stronger result is known, namely the Minkowski determinant theorem [5, p. 115].) Using this fact, the definition of (H/H_{11}), and the lemma, we see

$$\det H_{22} \geq \det (H/H_{11}) + \det H_{12}^* H_{11}^{-1} H_{12}. \tag{2}$$

(Clearly, (2) is equality when $k=1$.) Multiplication of (2) by $\det H_{11}$ yields the result.

We proceed to use Theorem 1 to analyze Hadamard's theorem.

THEOREM 2: *Let* H *be positive definite hermitian. Suppose* u_t *is the row vector* $(\mathrm{h}_{t,1}, \ldots, \mathrm{h}_{t,t-1})$, *and* H_t *is the leading* $\mathrm{t}\times\mathrm{t}$ *principal submatrix of* H. *Then*

$$h_{tt} - u_t H_{t-1}^{-1} u_t^* > 0$$

and

$$h_{11} \prod_{t=2}^{n} (h_{tt} - u_t H_{t-1}^{-1} u_t^*) = \det H.$$

In a certain sense, Theorem 2 gives the final word on the Hadamard theorem. It shows just what is being thrown away to obtain the inequality.

PROOF: The proof is by induction on n. From Theorem 1 (with $k=1$),

$$\det H_{n-1}(h_{nn}-u_nH_{n-1}^{-1}u_n^*)=\det H.$$

But, $\det H_{n-1}, \det H>0$. Hence $(h_{nn}-u_nH_{n-1}^{-1}u_n^*)>0$. By induction,

$$\det H_{n-1}=h_{11}\prod_{t=2}^{n-1}(h_{tt}-u_tH_{t-1}^{-1}u_t^*)$$

and $(h_{tt}-u_tH_{t-1}^{-1}u_t^*)>0$.

(Alternatively, one can prove, using the Laplace expansion theorem [5, p. 14], that

$$\frac{\det H_t}{\det H_{t-1}}=h_{tt}-u_tH_{t-1}^{-1}u_t^*.)$$

Using different methods, Marcus and Soules [6] obtained Theorem 1 for the case $k=1$. They also obtained an analog of it for the permanent. They used their result to prove Theorems 3 and 4 (below) but failed to notice Theorems 2 and 5.

THEOREM 3: *Let* H *be positive definite hermitian. Let* u_t *and* H_t *be as in Theorem* 2. *Then*

$$\prod_{t=1}^{n}h_{tt}-\det H=(\det H_{n-1})u_nH_{n-1}^{-1}u_n$$

$$+\sum_{k=2}^{n-1}\left(\prod_{j=n-k+2}^{n}h_{jj}\right)(\det H_{n-k})(u_{n-k+1}H_{n-k}^{-1}u_{n-k+1}^*).$$

The proof is an easy induction on n.

THEOREM 4: *Let* H *be positive definite hermitian with minimum eigenvalue* μ. *Then*

$$\prod_{t=1}^{n}h_{tt}-\det H\geqslant\mu^{n-2}\sum_{i<j}|h_{ij}|^2.$$

PROOF: Let ρ_{n-k} be the largest eigenvalue of H_{n-k}. Cauchy's inequalities [5, pp. 119] yield

(i) $\prod_{t=n-k+2}^{n}h_{tt}\geqslant\mu^{k-1}$,

(ii) $\det H_{n-k}\geqslant\rho_{n-k}\mu^{n-k-1}$,

(iii) $u_{n-k+1}H_{n-k}^{-1}u_{n-k+1}^*\geqslant\rho_{n-k}^{-1}\|u_{n-k+1}\|^2$.

The result follows from (i), (ii), (iii), and Theorem 3.

THEOREM 5: *Let* H *be positive definite hermitian with largest eigenvalue* ρ. *Then*

$$\prod_{t=1}^{n}h_{tt}-\det H\geqslant\frac{\det H}{\rho^2}\sum_{i<j}|h_{ij}|^2. \tag{3}$$

PROOF: For $1\leqslant k\leqslant n$, let $H(k)$ denote the submatrix of H obtained by deleting row and column k. Then

(i) $\left(\prod_{i=n-k+2}^{n} h_{ii}\right) \det H_{n-k} \geq \det H(n-k+1)$,

(ii) $\det H(n-k+1) \geq \rho^{-1} \det H$,

(iii) $u_{n-k+1} H_{n-k}^{-1} u_{n-k+1}^{*} \geq \rho^{-1} \|u_{n-k+1}\|^2$.

Number (i) follows by induction on Fischer's inequality or from Schur's theorem. Numbers (ii) and (iii) follow from Cauchy's inequalities. The result follows from (i), (ii), (iii), and Theorem 3.

Theorem 5 can be restated as

THEOREM 5′: *Let* $\lambda_1, \ldots, \lambda_n$ *be the eigenvalues of the positive definite matrix* H. *Then*

$$\prod_{i=1}^{n} \left(\frac{h_{ii}}{\lambda_i}\right) - 1 \geq \frac{1}{2\rho^2} \sum_{i=1}^{n} (\lambda_i^2 - h_{ii}^2) \geq 0.$$

PROOF: Divide (3) by $\det H = \lambda_1 \cdots \lambda_n$ and observe that

$$2 \sum_{i<j} |h_{ij}|^2 + \sum_{i=1}^{n} h_{ii}^2 = \text{trace } H^2 = \sum_{i=1}^{n} \lambda_i^2.$$

The author is pleased to acknowledge helpful discussions with Alan Goldman.

Note Added in Proof: It has been pointed out to me that theorem 1 was proved by Frederic T. Metcalf, A Bessel-Schwarz inequality for Gramiams and related bounds for determinants, Ann. Mat. Pura ed Appl. **68,** 201–232 (1965), corollary 10.2.

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On the Smith Normal Form

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An elementary proof is given of the fact that if A, B are nonsingular $n \times n$ matrices over a principal ideal ring R, then the kth invariant factor of AB is divisible by the kth invariant factor of A and by the kth invariant factor of B, $1 \leq k \leq n$. Some consequences are drawn.

Key words: Invariant factors; principal ideal rings, Smith normal form.

1. Introduction

Let R be a principal ideal ring (a commutative ring with identity 1 in which every ideal is principal). If $A \in R_n$ (the ring of $n \times n$ matrices over R) A^T will denote its transpose. If in addition A is nonsingular then

$$S(A) = \text{diag}(s_1(A), s_2(A), \ldots, s_n(A))$$

will denote the Smith normal form of A (see [2] for an excellent reference on this topic). It is well-known that if A, B are nonsingular elements of R_n then the determinantal divisors of AB are divisible by the corresponding determinantal divisors of A and of B. It is not so well-known that the same result is true for the invariant factors: i.e., $s_k(AB)$ is divisible by $s_k(A)$ and by $s_k(B)$, $1 \leq k \leq n$. An interesting consequence is that $S(AB) = S(A)S(B)$, provided that A, B have relatively prime determinants. This result is a consequence of a rather general theorem about rings which is given by Kaplansky in his paper [1].[1] Since Kaplansky did not include a proof of his theorem in his paper, and since the proof at any rate would be ring-theoretic, it is desirable to have a purely elementary matrix-theoretic proof, and this is what is given here.

We also note that the result concerning the determinantal divisors follows as a corollary, since if A is nonsingular then its kth determinantal divisor $d_k(A)$ is just $s_1(A)s_2(A) \ldots s_k(A)$, $1 \leq k \leq n$.

2. A Lemma

We first prove the following lemma:

LEMMA 1: *Suppose that* $\begin{pmatrix} H & 0 \\ 0 & K \end{pmatrix}$ *is a nonsingular element of* R_n *which is in Smith normal form. Let* m *be any non-zero element of* R *and suppose that there is a matrix* U *of* R_n *such that* (det U, m) = 1, *and*

$$U\begin{pmatrix} H & 0 \\ 0 & K \end{pmatrix} \equiv \begin{pmatrix} * & * \\ 0 & 0 \end{pmatrix} \bmod m. \tag{1}$$

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[1] Figures in brackets indicate the literature references at the end of this paper.

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Then K $\equiv 0 \bmod$ m.

PROOF: Put

$$H=\text{diag}\ (h_1, h_2, \ldots, h_r),\ K=\text{diag}\ (k_1, k_2, \ldots, k_s),$$

where $r+s=n$ and $h_i|h_{i+1}\ (1\leq i\leq r-1)$, $k_j|k_{j+1}\ (1\leq j\leq s-1)$, $h_r|k_1$. Partition U so that

$$U=\begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix},$$

where U_1 is $r\times r$, U_4 $s\times s$. Then (1) implies that

$$U_3H\equiv 0 \mod m, \tag{2}$$

$$U_4K\equiv 0 \mod m. \tag{3}$$

We can multiply (2) on the right by diag $(h_r/h_1, h_r/h_2, \ldots, 1)$ to obtain

$$h_rU_3\equiv 0 \mod m.$$

Put

$$(h_r, m)=\delta. \tag{4}$$

Then

$$\frac{h_r}{\delta}U_3\equiv 0 \mod \frac{m}{\delta},$$

and since $(h_r/\delta, m/\delta)=1$,

$$U_3\equiv 0 \mod \frac{m}{\delta}. \tag{5}$$

Now set $K=k_1K'$, where $K'=\text{diag}\ (1, k_2/k_1, \ldots, k_s/k_1)$. Then from (3),

$$k_1U_4K'\equiv 0 \mod m.$$

Put

$$(k_1, m)=\Delta. \tag{6}$$

Then as before we deduce that

$$U_4K'\equiv 0 \mod \frac{m}{\Delta}. \tag{7}$$

Now $\delta|\Delta$, in virtue of (4), (6), and the fact that $h_r|k_1$. It follows that $m/\Delta|m/\delta$, and so (5) holds modulo m/Δ as well. Thus

$$U=\begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}\equiv\begin{pmatrix} U_1 & U_2 \\ 0 & U_4 \end{pmatrix} \mod \frac{m}{\Delta},$$

$$\det U\equiv \det U_1 \det U_4 \bmod \frac{m}{\Delta}.$$

Since $(\det U, m) = 1$, it follows that $(\det U_4, m/\Delta) = 1$. Hence (7) implies that $K' \equiv 0 \bmod m/\Delta$, and so $\Delta \equiv 0 \bmod m$, since the 1,1 element of K' is 1. Thus (6) implies that $m | k_1$, and the conclusion follows.

3. The Theorems

We are now prepared to use Lemma 1. Let A, B be nonsingular elements of R_n. Then matrices U, C of R_n exist such that U is a unit matrix and

$$US(AB) = S(A)C. \tag{8}$$

Certainly $s_1(A)$ divides $s_1(AB)$, since $s_1(A)$ is the greatest common divisor of the elements of A and $s_1(AB)$ the greatest common divisor of the elements of AB. For $2 \leq k \leq n-1$, choose $m = s_k(A)$ and apply Lemma 1. We are left with $k = n$. Write $U = (u_{ij})$, $C = (c_{ij})$. Then (8) implies that

$$u_{ij} s_j(AB) = c_{ij} s_i(A),$$

so that for $i = n$,

$$u_{nj} s_j(AB) \equiv 0 \bmod s_n(A).$$

Since $s_j(AB) \mid s_n(AB)$, $1 \leq j \leq n$, this implies that

$$u_{nj} s_n(AB) \equiv 0 \bmod s_n(A).$$

The fact that $s_n(A) \mid s_n(AB)$ now follows, since $(u_{n1}, u_{n2}, \ldots, u_{nn}) = 1$.

If we note that in addition $S(A^T) = S(A)$, the entire argument may also be applied to the pair B^T, A^T, and we finally obtain

THEOREM 1: *Let* A, B *be nonsingular elements of* $\mathrm{R_n}$. *Then* $\mathrm{s_k(AB)}$ *is divisible by* $\mathrm{s_k(A)}$ *and by* $\mathrm{s_k(B)}$ *for* $1 \leq \mathrm{k} \leq \mathrm{n}$.

From this theorem we easily deduce

THEOREM 2: *Suppose that* A, B *are elements of* $\mathrm{R_n}$ *with relatively prime determinants. Then*

$$\mathrm{S(AB) = S(A)S(B).}$$

PROOF: Since $(\det A, \det B) = 1$ and $s_k(A) \mid \det A$, $s_k(B) \mid \det B$, it follows that $(s_k(A), s_k(B)) = 1$ for $1 \leq k \leq n$. Then Theorem 1 implies that

$$s_k(AB) \equiv 0 \bmod s_k(A) s_k(B), \quad 1 \leq k \leq n.$$

But $\prod_{k=1}^{n} s_k(AB)$ is a unit multiple of $\det(AB)$, and $\prod_{k=1}^{n} s_k(A) s_k(B)$ is a unit multiple of $\det A \det B$. It follows that $s_k(AB) | s_k(A) s_k(B)$ is a unit for $1 \leq k \leq n$. But this implies that in fact $s_k(AB) = s_k(A) s_k(B)$ for $1 \leq k \leq n$, since associated elements in corresponding diagonal positions of matrices in Smith normal form must be equal. This completes the proof.

4. Concluding Remarks

Theorem 2 is definitely false if $(\det A, \det B) > 1$. Thus if m is any element of R, and

$$A = \begin{pmatrix} 1 & 1 \\ 0 & m \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 \\ -1 & m \end{pmatrix},$$

then

$$S(A) = S(B) = \begin{pmatrix} 1 & 0 \\ 0 & m \end{pmatrix},$$

but

$$S(AB) = \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}.$$

This example also shows that $S(AB)$ need not equal $S(BA)$, since here

$$S(BA) = \begin{pmatrix} 1 & 0 \\ 0 & m^2 \end{pmatrix}.$$

However, $S(AB)$ and $S(BA)$ are equal if A and B have relatively prime determinants as is readily seen from Theorem 2.

A simple example illustrating the use to which Theorem 1 may be put is furnished by choosing A as the incidence matrix of a finite projective plane of order n, so that A is a $v \times v$ rational integral matrix satisfying

$$AA^T = A^TA = nI + J,$$

where $v = n^2 + n + 1$ and J is the matrix all of whose entries are 1. It is easy to show that the invariant factors of $nI + J$ are

$$1(\text{once}),\ n(v - 2 \text{ times}),\ n(n+1)^2(\text{once}).$$

Thus if the Smith normal form of A is

$$S(A) = \text{diag } (\alpha_1, \alpha_2, \ldots, \alpha_v),$$

then

$$\alpha_1 = 1,\ \alpha_i | n (2 \leq i \leq v-1),\ \alpha_v | n(n+1)^2.$$

Now the facts that

$$\alpha_1\alpha_2 \ldots \alpha_v = n^{\frac{v-1}{2}} (n+1),$$

and $(\alpha_i, n+1) = 1$ for $1 \leq i \leq v-1$, imply that $\alpha_v = (n+1)\alpha_v'$, where now

$$\alpha_1\alpha_2 \ldots \alpha_{v-1}\alpha_v' = n^{\frac{v-1}{2}},$$

$$\alpha_i | \alpha_{i+1} (1 \leq i \leq v-2),\ \alpha_{v-1} | \alpha_v',\ \alpha_v' | n.$$

Choosing n square-free, we easily obtain

COROLLARY 1: *Let* A *be the incidence matrix of a finite projective plane of order* n, *where* n *is square-free. Then the invariant factors of* A *are*

$$1\left(\frac{n^2+n}{2} + 1 \textit{ times}\right),\ n\left(\frac{n^2+n}{2} - 1 \textit{ times}\right),\ n(n+1)\,(\textit{once}).$$

Of course such a matrix is known to exist only if n is a prime, and this result might possibly be of some use in settling the question of existence for other square-free values of n.

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On Certain Optimal Quadrature Formulas

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A class of optimal quadrature formulas defined by V. L. N. Sarma in a probabilistic context is shown to be identical with a class of formulas defined previously, in a different manner, by P. J. Davis. As a result a contrast is drawn between the maximum of the error of a quadrature fomula over the unit sphere in a certain function space, and its average—in Sarma's sense—over that sphere.

Key words: Analytical functions; approximation; Gaussian quadrature; integration; optimal quadrature; quadrature.

A few years ago V. L. N. Sarma [1][1] defined a probability measure on a certain space of functions and proposed that quadrature formulas be studied in terms of their average error on this space. If

$$Q(f)=Q_N(f)=\sum_{r=1}^{N} a_r f(x_r) \tag{1}$$

is any N-point quadrature formula, and $E^Q(f)=I(f)-Q(f)$ where $I(f)$ is the integral which Q is approximating, we shall denote by "$\sigma(E^Q)$" the "RMS" average of E^Q with respect to Sarma's measure. Sarma calls a formula Q_N "completely optimal" if $\sigma(E^{Q_N}) \leq \sigma(E^{Q'_N})$ for every N-point formula Q'_N; and he calls it "optimal in the weights" if $\sigma(E^{Q_N}) \leq \sigma(E^{Q'_N})$ for every N-point Q'_N using the same points $x_1, x_2, \ldots, x_N$. It is the purpose of this note to point out that, in the case of integration of functions of one variable, Sarma's optimal formulas are identical with those defined earlier by P. J. Davis in a quite different manner; and to discuss some consequences of this identity.

In the one-variable case, Sarma's space consists of all those functions analytic in the open unit disk whose Taylor series

$$f(z)=\sum_{n=0}^{\infty} a_n z^n \tag{2}$$

satisfy the condition

$$\sum_{n=0}^{\infty} |a_n| = 1. \tag{3}$$

The integral considered is

$$I(f)=\int_{-1}^{1} f(x)dx; \tag{4}$$

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[1] Figures in brackets indicate the literature references at the end of this paper.

and he showed that the average error σ is given by the formula

$$\sigma^2(E^Q) = \sum_{n=0}^{\infty} 3^{-n-1} (E^Q(x^n))^2 \tag{5}$$

([1], p. 610).

In 1953, P. J. Davis [2] introduced another measure of quadrature error for analytic functions. In the notation of [3], Davis considers the integral (4) for f belonging to the Hilbert Space $H^2(C_R)$: the space of all those functions analytic in the disk $|z| < R$ (where R is any number > 1) whose Taylor series satisfy the condition

$$\sum_{n=0}^{\infty} |a_n|^2 R^{2n} < \infty. \tag{6}$$

The inner product is defined by

$$(f, g)_R = 2\pi R \sum_{n=0}^{\infty} a_n \bar{b}_n R^{2n} = \int_{C_R} f(z)\overline{g(z)}ds \tag{7}$$

where a_n and b_n are the Taylor coefficients of f and g respectively and C_R is the circle $|z| = R$; s denotes arc length. For any Q of the form (1), with quadrature points x_r inside C_R, E^Q turns out to be a bounded linear functional, and its norm is given [3] by

$$\|E^Q\|_R^2 = \frac{1}{2\pi R} \sum_{n=0}^{\infty} R^{-2n} (E^Q(x^n))^2. \tag{8}$$

A knowledge of this norm affords us the error bound

$$|I(f) - Q(f)| \leq \|E^Q\| \cdot \|f\|;$$

and Davis defined optimality of quadrature formulas in the same manner as Sarma, with the norm $\|E^Q\|$ in place of $\sigma(E^Q)$.

Comparison of (5) and (8) shows that

$$\sigma(E^Q) = \left(\frac{2\pi}{3^{1/2}}\right)^{1/2} \|E^Q\|_{\sqrt{3}}; \tag{9}$$

since the two measures of E^Q differ by a constant factor, it follows that the quadrature formulas optimal in Sarma's sense are precisely those optimal in Davis' sense for the space H^2 $(C_{\sqrt{3}})$.

The H^2 spaces have many convenient analytic properties, and the norms $\|E^Q\|_R$ have been studied for various Q's ([4], [5]). In [3] I showed that for $Q = G_N$ — the N-point Gauss-Legendre quadrature formula (for a description of these formulas see, e.g., [6], chap. 8) — we have the bound

$$\|E^{G_N}\|_R \leq A \sqrt{2N+1}\, \rho^{-N} \tag{10}$$

where

$$\rho = 2R^2 - 1 + 2R(R^2-1)^{1/2} \tag{11}$$

and

$$A = 32 e^{1/2} \pi^{-3/2} \rho^{-1/4} \left(\frac{\rho^{1/2} + \rho^{-1/2}}{\rho^{1/2} - \rho^{-1/2}}\right)^{1/2}. \tag{12}$$

If $R=\sqrt{3}$, then $\rho=5+2\sqrt{6}$, and it follows that $||E^{G_N}||_{\sqrt{3}}$ goes to zero about as fast as $(0.1010)^N$, or faster. In a recent paper [7], Sarma and A. H. Stroud calculated $\sigma(E^{G_N})$ for $N=2, 3, 4, \ldots, 20$, and observed that $\sigma(E^{G_N})/\sigma(E^{G_{N-1}})$ was very close to 0.10. Because of the relation (9), this ratio is the same as

$$||E^{G_N}||_{\sqrt{3}} \; / ||E^{G_{N-1}}||_{\sqrt{3}},$$

and these data seem to indicate that the left side of (10) does, indeed, give about the right rate of decrease for $||E^{G_N}||_R$.

(Sarma and Stroud remark that $\sigma(E^{G_N})/\sigma(E^{G_{N-1}})$ appears to be approaching 0.1 as $N\to\infty$. A closer look at their data suggests that the limit is somewhat higher. If one calculates the first differences of the successive values of $\sigma(E^{G_N})/\sigma(E^{G_{N-1}})$, it is seen that these differences are positive and decreasing, and the ratios of successive differences are increasing. If this behavior continues for higher N, $\sigma(E^{G_N})/\sigma(E^{G_{N-1}})$ must eventually become greater than

$$\sigma(E^{G_{20}})/\sigma(E^{G_{19}})+\Delta_{20}\left[\left(\frac{\Delta_{20}}{\Delta_{19}}\right)+\left(\frac{\Delta_{20}}{\Delta_{19}}\right)^2+\left(\frac{\Delta_{20}}{\Delta_{19}}\right)^3+\ldots\right], \tag{13}$$

where

$$\Delta_N=\sigma(E^{G_N})/\sigma(E^{G_{N-1}})-\sigma(E^{G_{N-1}})/\sigma(E^{G_{N-2}}).$$

The quantity (13) is greater than 0.1003; so it appears that the Sarma-Stroud data are consistent with the ratio of the σ's approaching $(5+2\sqrt{6})^{-1}$).

It is interesting to compare Sarma's σ with a very directly related error bound. Following Sarma, let S be the space of all those functions analytic in the open unit disk whose Taylor series (2) satisfy

$$\sum_{n=0}^{\infty}|a_n|<\infty, \tag{14}$$

and define

$$||f||_S=\sum_{n=0}^{\infty}|a_n|. \tag{15}$$

S is a Banach Space, isomorphic to the space l_1 of absolutely convergent series of complex numbers. Sarma's $\sigma(E^Q)$ is a root-mean-square average of E^Q over the unit sphere in S. In contrast, the norm of E^Q—regarded as a functional on S—is the supreme of $|E^Q|$ on the same unit sphere. This norm, which I shall denote by "$||E^Q||_S$" allows the error bound

$$|I(f)-Q(f)|\leq||E^Q||_S\cdot||f||_S, \qquad f\epsilon S. \tag{16}$$

In the spirit of Davis' approach, $||E^Q||_S$ would be used in place of $\sigma(E^Q)$. Let us compare the sizes of these two quantities:

For every $R>1$, if $f\epsilon H^2(C_R)$ then $f\epsilon S$; and if we write

$$||f||_R=(f,f)_R^{1/2}=\left\{2\pi R\sum_{n=0}^{\infty}|a_n|^2R^{2n}\right\}^{1/2}, \tag{17}$$

we may compare $||f||_R$ and $||f||_S$. Setting $b_n=|a_n|R^n$, we have

$$\left(\sum_{n=0}^{\infty}|a_n|\right)^2=\left(\sum_{n=0}^{\infty}b_nR^{-n}\right)^2$$

$$\leq\left(\sum_{n=0}^{\infty}b_n^2\right)\left(\sum_{n=0}^{\infty}R^{-2n}\right)$$

$$\leq \frac{R^2}{R^2-1}\sum_{n=0}^{\infty} b_n^2$$

by the Schwartz inequality; and it follows that

$$\|f\|_S \leq K(R)\|f\|_R \tag{18}$$

where

$$K(R) = \left(\frac{R}{2\Pi(R^2-1)}\right)^{1/2}. \tag{19}$$

Therefore

$$\|E^Q\|_S = \sup_{f\in S} \frac{|E^Q(f)|}{\|f\|_S}$$

$$\geqslant \sup_{f\in S} \frac{|E^Q(f)|}{K(R)\|f\|_R}$$

$$\geqslant \frac{1}{K(R)} \sup_{f\in H_2(C_r)} \frac{|E^Q(f)|}{\|f\|_R}$$

$$\geqslant \frac{1}{K(R)} \|E^Q\|_R. \tag{20}$$

The experimental evidence seems to indicate that, for $Q = G_N$, the asymptotic behavior of $\|E^{G_N}\|_R$ for large N is correctly given (at least to within factors like N^a) by the right side of (10). If this is so, then (20) shows that $\|E^{G_N}\|_S \neq 0(C^{-N})$ for any $C > 1$, while (by (9), (10), and (11)) $\sigma(E^{G_N}) = 0(3^{-N}N^{1/2})$. Equation (16) may be a very conservative bound; in numerical experiments [8] an analogous bound has been found to be considerably larger than the actual quadrature error. Since Sarma's "average error" $\sigma(E^{G_N})$ appears to be very much smaller than the right side of (16), it would be interesting to know whether it does, indeed, represent the "average" behavior of quadrature formulas for the integrands arising in the course of practical numerical work. I do not see how to answer this question.

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Publications of the National Bureau of Standards*

Other NBS Publications

Greenberg, L., Newman, M., **Some results on solvable groups,** *Arch. Math.* **21,** *No. 4, 349–352 (1970).*

Key words: Density; 2-generator groups; solvable groups.

Let a, b be fixed relatively prime integers > 1. Let $s(n) = 1$ if a solvable group of order n exists generated by elements x, y such that $x^a = y^b = 1$; and 0 otherwise. It is proved that

$$\frac{1}{x} \sum_{n \le x} s(n) \to 0 \text{ as } \quad x \to \infty.$$

J. Res. Nat. Bur. Stand. (U.S.), 75A (Phys. and Chem.), No. 1 (Jan.–Feb. 1971), SD Catalog No. C13.22/sec.A:75/1. $1.25.

High-speed (subsecond) measurement of heat capacity, electrical resistivity, and thermal radiation properties of tantalum in the range 1900 to 3200 K. A. Cezairliyan, J. L. McClure, and C. W. Beckett.

Thermophysical properties of methane: orthobaric densities and some thermal properties. R. D. Goodwin.

The infrared spectrum of matrix isolated BaO_2. S. Abramowitz and N. Acquista.

Refinement of the crystal structure of the aragonite phase of $CaCO_3$. B. Dickens and J. S. Bowen.

Simple shearing flows in polyisobutylene solutions. L. J. Zapas and J. C. Phillips.

Synthesis of fluorodienes. J. E. Fearn.

Quantum corrections to the second virial coefficient for the Lennard-Jones $(m-6)$ potential. M. E. Boyd.

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